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March 6, 2006

Dr. Anil E. Deane
Program Manager
SC-20/Germantown Building
U.S. Department of Energy
1000 Independence Ave., S.W.
Washington, DC 20585-1290

ATTN: Program Announcement LAB 06-04, Scientific Discovery Through Advanced Computing

Dear Dr. Deane :

Accompanying this letter is a grant proposal titled "Statistical Approaches to Aerosol Dynamics for Climate Simulation," prepared by Dr. Robert L. McGraw of Brookhaven National Laboratory and Professor Wei Zhu of the State University of New York at Stony Brook.

This collaborative proposal is a Science Application Partnership (SAP) submitted in response to Notice DE-FG02-06ER06-04, Scientific Discovery through Advanced Computing (SciDAC). This proposed (SAP) is an integral part of the inter-Laboratory proposal: "A scalable and Extensible Earth System Model for Climate Change Science," submitted under this SciDAC call (PI: John Drake of ORNL). The funding requested is part of that proposals OASCR SAP request.

If you require additional information regarding the proposal, please contact Dr. McGraw at 631-344-3086.

Sincerely,

Ralph James
Ralph James
Associate Laboratory Director for
Energy, Environment, and National Security

Enclosures
c: A. S. Bamzai, DOE
M. Holland, DOE Site Office

U. S. DEPARTMENT OF ENERGY
FIELD WORK PROPOSAL

1. B&R No.	2. Contractor No.: EE-619-EECA	3. Date Prepared: 03/06/2006	4. Task Term: Begin: 07/01/2006 End: 06/30/2009

5. Work Proposal No.:	6. Work Authorization No.:

7. Title: Statistical Approaches to Aerosol Dynamics for Climate Simulation

8. Principal Investigator(s) : Robert McGraw (631) 344-3086

9. Headquarters/Operations Office Program Manager: Petty, Rickey C. (301) 903-5548	12. Headquarters Organization: Office of Science	15. HQ Organizational Code: SC
10. Operations Office Work Proposal Reviewer:	13. Operations Office: CHICAGO	16. DOE Organizational Code: CH
11. Contractor Work Proposal Manager: Daum, Peter H. (631) 344-7283	14. Contractor Name: BROOKHAVEN SCIENCE ASSOCIATES BROOKHAVEN NATIONAL LABORATORY	17. Contractor Code: BN

18. Work Proposal Description (Approach, anticipated benefit in 200 words or less, suitable for public release) :

The quadrature method of moments (QMOM), developed in recent years in collaborations between Brookhaven National Laboratory (BNL) scientists and The State University of New York at Stony Brook (SUNY-SB) mathematicians, provides a statistically-based alternative to modal and sectional methods for aerosol simulation. Key moments of the aerosol population, including number, mass, and mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. The new approach is highly efficient, yet provides the comprehensive representation of natural and anthropogenic aerosols, and of their mixing states and direct and indirect effects, that the Community Climate System Model (CCSM) will require. If it pans out as expected, it will be an attractive option for handling aerosols for the following Intergovernmental Panel on Climate Change assessment (AR6). In addition to furthering its partnership with SUNY-SB, the proposed Science Application Partnership will leverage findings from current BNL science programs related to aerosols [Department of Energy/Atmospheric Sciences Program (DOE/ASP)], aerosol-cloud interaction [DOE/Atmospheric Radiation Measurement (ARM)], and climate simulation [National Aeronautics and Space Administration-Goddard Institute for Space Studies] to the maximum extent possible to meet Climate Change Prediction Program objectives in collaboration with the inter-laboratory science team.

Keywords: aerosol dynamics, quadrature method of moments, atmospheric aerosols, climate simulation

19. Principal Investigator (s) :

Robert McGraw — 03/06/2006

Signature(s) — Date

20. Contractor Work Proposal Manager:

P. Daum (by C. D. Wil...) — 03/06/2006

Signature — Date

21. Operations Office Review Official:

Signature — Date

22. Detail Attachments:

- (☒) a. Purpose
- (☒) b. Approach
- (☒) c. Technical progress
- (☒) d. Future accomplishments
- (☒) e. Relationships to other projects
- (☐) f. Explanation of milestones
- (☐) g. Other (Specify Topic)

22. Detailed Attachments

a. Purpose

- Develop new statistical approaches for improving the representation of aerosols, aerosol microphysical processes, and aerosol-cloud interactions in the CCSM; and,

- Supply a new aerosol module based on these findings in time for CCSM5.

This work effort may support, at a minimum level or concurrently as appropriate, the Technology Transfer and Science Education missions of the DOE.

b. Approach

BNL will participate in the activities of this proposal in partnership with the Department of Applied Mathematics and Statistics (AMS) of SUNY-SB. Specifically, BNL will contribute to the Earth Simulation Model currently being proposed by an inter-Laboratory science application team on which BNL is a participant. BNL will participate through the activities of this proposal by way of three tasks:

(1) Developing new capabilities for aerosol simulation using advanced statistical methods and improvements to the QMOM;

(2) Leveraging of findings from its current DOE ASP and DOE ARM science programs related to aerosols and aerosol-cloud interactions, especially for development of new parameterizations suitable for use in the CCSM; and,

(3) Supplying a new aerosol module based on the new methods.

To successfully carry out these activities the BNL Atmospheric Sciences Division will lead the science application work and build on an already successful collaboration with the AMS Department at SUNY-SB, which will lead the mathematical development.

Key Personnel: Robert L. McGraw (BNL), Wei Zhu (SUNY-SB)

c. Technical Progress

This is a new proposal that is being prepared for submission March 6, 2006.

d. Future Accomplishments

Expected Progress in Year 1

Continue development of multivariate extensions of the QMOM. Selection of optimal moment sets for multi-component aerosols. Development of new statistical approaches for the systematic classification of aerosol mixing states. Initiate construction of QMOM module and incorporation of microphysical parameterizations.

Expected Progress in Year 2

Apply Visual Statistical Analyzer framework methods, developed for classification of field aerosol measurements, to optimize modal (class) structures for aerosol simulation. Apply Bayesian statistical methods to the characterization of evolving aerosol populations. Begin benchmark validations of the QMOM aerosol module using high-resolution sectional and analytic methods.

d. Future Accomplishments (cont.)

Expected Progress in Year 3

Completion of QMOM module validation studies. Prepare for integration into the CCSM.

e. Relationships to Other Projects

The activities of this program are directly coupled to other DOE-funded programs at BNL as well as to other activities at other laboratories participating in the DOE ASP and in the DOE ARM program. BNL is a part of the DOE ASP program: New particle formation: Mechanisms and influence on atmospheric aerosol properties. It is also part of the DOE ASP program: Modeling Aerosol Processes in the DOE Atmospheric Science Program. Parameterizations developed for new particle formation, for water uptake with changes in relative humidity, and for sea salt aerosol production flux developed under these programs will be leveraged to meet needs of the proposed study. BNL is a part of the DOE ARM program: Developing new theory and parameterizations for clouds and precipitation in climate models. It is also part of the DOE ARM program: Aerosol Cloud Interactions: Field Studies and Interpretation. Parameterizations for aerosol-cloud interactions and indirect effects, including drizzle formation, developed under these programs will be leveraged to meet needs of the proposed study.

BROOKHAVEN NATIONAL LABORATORY

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Environmental Sciences Department
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Operated by
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with the
U.S. Department of Energy

Statistical Approaches to Aerosol Dynamics for Climate Simulation

A Proposal Submitted to

Office of Science
Scientific Discovery through Advanced Computing (SciDAC) Lab 06-04

March 6, 2006

Funding: Year 1: $315,093; Year 2: $326,857; Year 3: $337,493; Total: $979,443

There is no use of human subjects in this proposed project.
There is no use of Vertebrate animals in this proposed project.

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Table of Contents

1. Abstract

The quadrature method of moments (QMOM), developed in recent years in collaborations between BNL scientists and SUNY-SB mathematicians, provides a statistically-based alternative to modal and sectional methods for aerosol simulation. Key moments of the aerosol population, including number, mass, and mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. The new approach is highly efficient, yet provides the comprehensive representation of natural and anthropogenic aerosols, and of their mixing states and direct and indirect effects, that the CCSM will require. In addition to furthering its partnership with SUNY-SB, the proposed SAP will leverage findings from current BNL science programs related to aerosols (DOE ASP), aerosol-cloud interaction (DOE ARM), and climate simulation (NASA-GISS) to the maximum extent possible to meet CCPP objectives in collaboration with the inter-laboratory science team.

2. Background

2.1 Objectives

The goal of the DOE Climate Change Prediction Program (CCPP), including the SciDAC Climate Modeling and Simulation Science Application, is:

• *To determine the range of possible climate changes over the 21st century and beyond through simulations using a more accurate climate system model that includes the full range of human and natural climate feedbacks with increased realism and spatial resolution.*

This Science Application Partnership (SAP) will support that goal through its development of statistically-based approaches to aerosol simulation. These approaches tend to be highly efficient and will contribute to maximizing the length of simulations and number of ensembles that can be performed to facilitate the aggressive schedule of climate change simulations required for upcoming assessment products. This SAP has been called out in the inter-Laboratory science application proposal: "A Scalable and Extensible Earth System Model for Climate Change Science", submitted under this SciDAC call (PI: John Drake of ORNL) and will contribute in an integral way to that proposed activity. Indeed this is the only SAP called out as part of that inter-Laboratory proposal to improve the representation of aerosols in the Community Climate System Model (CCSM).

The specific objectives of the proposed SAP can be summarized as follows:

• *To develop new statistical approaches for improving the representation of aerosols, aerosol microphysical processes, and aerosol-cloud interactions in the CCSM.*

• *To supply a new aerosol microphysical module based on these findings in time for CCSM5.*

2.2 Significance

In contrast to greenhouse gases, radiative forcing by aerosols cannot be characterized simply by mass concentration as has been employed in many past and current evaluations (Schmidt et al., 2006). Rather, the direct effects of aerosol on atmospheric radiation strongly depend upon the sizes, shape, chemical composition, and mixing state of the particle distribution (Jacobson, 2001, 2002). Understanding the complex processes that shape this variability is a major scientific challenge (Asrar et al., 2001). Similarly, size-resolved simulations of aerosol microphysics, including number and mass concentrations are necessary to understanding and modeling the indirect effect of aerosols on clouds (Adams and Seinfeld, 2002). Anthropogenic aerosols are believed to have two effects on cloud properties: (1) The increase in the number of cloud condensation nuclei results in a larger number of smaller droplets and brighter clouds (the Twomey effect) (Schwartz et al., 2002), (2) The smaller droplets tend to inhibit rainfall increasing cloud lifetime and average cloud cover (Rosenfeld, 2000). These indirect effects of aerosol on clouds have been characterized as contributing perhaps the largest of all uncertainties about global climate forcings (NRC, 2001). It is thus imperative for future assessments of aerosol forcing that the aerosol number, size distribution, chemical composition, and mixing state be represented in models in sufficient detail to make accurate estimates of cloud activation and optical properties of the aerosol if the uncertainty that presently attaches to estimates of this forcing is to be appreciably reduced. The aerosol mixing state, for example, plays a major role in determining particle optical properties, solubility and cloud activation efficiency, yet has not been adequately represented in traditional aerosol models. These aerosol properties are likewise of great significance to the interpretation of ground based and remote sensing measurements.

As described below, we in the aerosol microphysics community have made considerable progress in developing the advanced methods and highly efficient modular components necessary to represent both the direct and indirect effects of aerosols in atmospheric models. It is thus timely and imperative for improved assessment of climate effects that these new developments be incorporated in the next generation Earth system model. The development of highly efficient size and composition resolved aerosol modules based on the quadrature method of moments (QMOM) affords a timely opportunity to fill this need, and specifically to update the representation of aerosols and their direct and indirect effects in the CCSM.

2.3 Relation to current state-of-the art

Traditional approaches to aerosol modeling have mainly centered on the use of "modal" and "sectional" methods. Modal methods typically divide the aerosol into a small number of modes of prescribed shape and having uniform composition within each mode. The method is efficient but generally not very accurate. Sectional methods divide the aerosol into a number of size classes. High accuracy requires good size resolution in order to minimize numerical diffusion, with the result that a large number of class variables (scalars) needs to be carried in the model. A high-resolution sectional calculation is useful, even vital, as a validation tool for off-line testing of more approximate methods, but is an unlikely candidate for use in climate simulation. Thus it is clear that new and efficient approaches are needed for the aerosols.

The method of moments, especially as developed over recent years in collaborations between BNL scientists and SUNY-SB mathematicians (Yoon and McGraw, 2004a; 2004b), provides a statistically-based alternative for aerosol simulation. The new approach is highly efficient and especially suited to simulations of the multicomponent aerosols that the CCSM will require. Key moments of the aerosol population, including number, mass, and the mixed moments entering the covariance matrix of a principal components analysis, are tracked in place of the distribution itself. This greatly reduces the number of aerosol scalars required by the model without compromising the accuracy with which the physical and optical properties of the aerosol are computed – properties computed directly from the moments. The quadrature method of moments (QMOM) has been advanced in recent years to the point where it is now widely regarded as an extremely accurate method and a viable alternative to bin-sectional and modal methods for describing the dynamics of particle populations in models. **The QMOM has a potential future with the CCSM: It is clearly more efficient than sectional and more accurate than modal methods.**

2.4 Preliminary Studies

This section presents an overview of some the more significant advances achieved in the representation of aerosols by the method of moments. Parameterizations to describe how aerosols activate to form cloud droplets (these set requirements on the aerosol module), and new results for parameterization of the autoconversion process governing the transition from cloud droplets to precipitation are also summarized.

2.4.1 The quadrature method of moments

Gaussian quadrature provides a systematic method for approximate evaluation of integrals of the form given by Eq. 2.1:

$$I = \int_0^\infty \sigma(r) f(r) dr \approx \sum_{i=1}^{N} \sigma(r_i) w_i \qquad (2.1)$$

where $\sigma(r)$ is a known kernel function, in this case a function of the particle radius. For our purpose the weight function, $f(r)$, is the aerosol size distribution, and *I*, depending on the nature of the kernel is some integral property of the distribution.

Two key properties of quadrature underlie the power of the QMOM: (1) for N quadrature points $\{r_i; w_i\}$ the approximate equality of Eq. 2.1 is exact for polynomial kernels of degree $2N - 1$, and (2) the quadrature abscissas and weights, $\{r_i\}$ and $\{w_i\}$, respectively depend only on the moments of $f(r)$:

$$\mu_k = \int_0^\infty r^k f(r) dr = \sum_{i=1}^{N} (r_i)^k w_i \qquad (2.2)$$

for $k = 0,1,2,\ldots,2N-1$. Thus one does not require full knowledge of $f(r)$ in order to evaluate integral properties of the aerosol as it suffices to know only the lower order moments. Efficient methods for obtaining quadrature abscissas and weights from moments have been developed for the univariate case, i.e. an aerosol distribution that, like $f(r)$ above, is specified using only a single particle radius (or mass) coordinate [See for example McGraw, 1997 or the Numerical Recipes subroutine OTHOG (Press et al., 1992)]. An important goal of the statistical approach is to develop methods for extending the assignment of quadrature points to multivariate particle distribution functions (pdfs) as described below in Sec. 3.

The physical and optical properties of an aerosol can be estimated from its moments using Eq. 2.1. Figure 1 illustrates a particularly difficult case where $\sigma(r)$ is the Mie-scattering angular distribution kernel at a single wavelength and in a particular scattering direction for a spherical particle of radius *r* (McGraw et al., 1995). The behavior of $\sigma(r)$ is shown at four scattering directions ranging from forward scattering ($\theta = 0$) to backscattering at 180°. The total scattering due to the aerosol, at any specified angle, is an integral of type *I* (Eq. 2.1). Property 1 gives an indication of the accuracy to expect. Thus if the kernel were a fifth-degree polynomial (solid curves in Fig. 1) the obtained result would be exact for *N*=3. The figure shows that the true kernels are indeed reasonably well fit by polynomials except in the 180° backscattering case where strong oscillations in the kernel are not captured well by the fit. Comparison of both sides of the approximate equality of Eq. 2.1 for representative known particle size distributions shows the method leads to nonsystematic errors in the range $\pm 5\%$, except in the 180° backscattering case where errors reached over 40%. Moreover, these results were for a single wavelength – the most unfavorable case. Many practical applications average over multiple wavelengths, as in the solar spectrum, and the errors tend to cancel to obtain much more accurate results. With further averaging over a vertical column of grid cells and multiple aerosol types (the reported results are for a single homogeneous aerosol) the error is even further reduced. The utility of moment methods for properties estimation has been enhanced by the development of methods such as Randomized Minimization Search Technique (RMST) and Multiple Isomomental Distribution Aerosol Surrogate (MIDAS), which use the first six moments to compute aerosol optical properties to within 1-2% of those obtained from the full particle distribution function (PDF) (Yue et al., 1997; Wright, 2000). These methods can be used even for pathologically non-polynomial kernels, such as the step function kernels often used in models of cloud droplet activation (Wright et al., 2002), although here a better approach would be to develop parameterizations for aerosol-cloud interaction directly in terms of moments (Sec. 3).

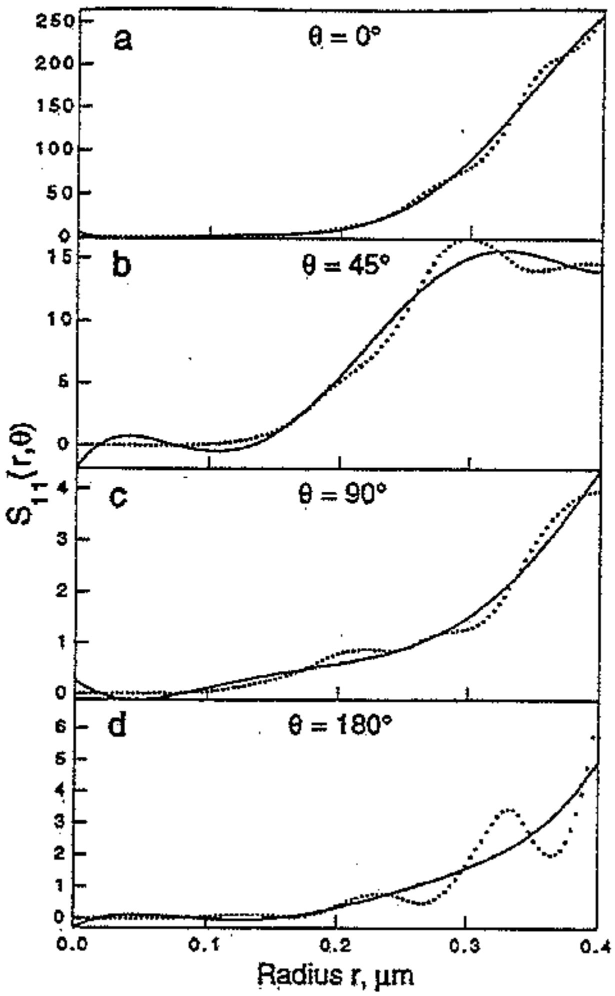

Figure 1. Mie scattering angular distributions (unnormalized). Dotted curves result from Mie scattering calculations at a wavelength of 0.6328µm. Solid curves are fifth-degree polynomial fits. To the extent that the Mie curves can be approximated by the corresponding polynomial forms the quadrature approximation of Eq. 2.1 is exact (from McGraw at al., 1995).

The quadrature approximation to integrals of type I, also leads to the moment closure necessary to simulate general aerosol evolution processes using only moments. We will illustrate this idea here for condensation growth. Results for other aerosol processes including coagulation, dry deposition, even cloud activation, follow in similar fashion. Let $dr/dt = \phi(r)$ be an arbitrary particle growth rate. Then from Eq. 2.1 (McGraw and Wright, 2003):

$$\frac{d\mu_k}{dt} = k\int_0^\infty r^{k-1}\phi(r)f(r)dr \approx k\sum_{i=1}^{N}(r_i)^{k-1}\phi(r_i)w_i . \qquad (2.3)$$

The abscissas and weights are the same as before – independent of kernel and dependent only on lower order moments. Equations 2.2 and 2.3 provide an example of closure for moment evolution equations that is the basis for the QMOM (McGraw, 1997).

These results have immediate consequences for simulation efficiency – i.e., one need not track the full aerosol distribution as just a few moment scalars are sufficient for obtaining aerosol physical and optical properties and closure of the moment dynamics. Moreover, approximations for estimating particle size distributions from moments have been developed and although the solutions are not unique the latest results are promising (Wright, 2000; Diemer and Olson, 2002).

2.4.2 Recent applications

Recent years have seen development of the QMOM to the point where it is now widely regarded as an extremely accurate method and a viable alternative to bin-sectional and modal methods for describing the dynamics of particle populations (see for example Marchisio et al., 2003a, 2003b and Upadhyay and Ezekoye, 2003 for independent assessments of QMOM accuracy in chemical engineering applications). A recent monograph includes a fifteen page appendix describing the QMOM and new applications including closure of the moment equations for turbulence, and especially for simulating particle population dynamics in turbulent flows (Fox 2003). Along similar lines, the QMOM is now available as a user specified option in the popular computational fluid dynamics code FLUENT (Wan et al., 2004).

Its remarkable efficiency makes the QMOM ideal for use in atmospheric models. The method has been used for the representation of aerosols in chemical transport models (CTMs) on the sub-hemispheric (Wright et al., 2000) and regional scales (Yu et al., 2003). As described above, the QMOM tracks key moments of the aerosol population directly, without need for a priori assumptions regarding the form of the particle size distribution, while overcoming difficulties associated with closure of the moment evolution equations encountered in the ordinary MOM. An early QMOM aerosol dynamics module 6M (for 6 radial moments) includes a range of aerosol microphysical and chemical processes and allows for arbitrary growth laws for condensation and coagulation, nucleation of new particles, and precursor gas and liquid-phase chemistry (Wright et al., 2001a; Yu et al., 2003). Comparison with results obtained using a high-resolution discrete model of the particle dynamics, demonstrated that the accuracy of 6M is good relative to uncertainties associated with other processes represented in atmospheric CTMs (Wright et al., 2001a). For example differences in the mass/volume moments and in the partitioning of chemical species such as sulfur (VI) between the gas and aerosol phases remained under 1% and differences in particle number rarely exceeded 15% (Wright et al., 2001a).

2.4.3 Multivariate extension of moment methods

In addition to particle mass loading, the chemical and physical properties of aerosols are determined by particle number density, composition, and size distribution. In the atmosphere, particle number and composition control the indirect effects that aerosols have on climate through their influence on cloud activation, drizzle production, and cloud radiative properties. Another example points to the mixing state of black carbon aerosols as having a significant influence on radiative forcing (Jacobson, 2001). Unlike the limiting cases of externally or internally mixed aerosols, the modeling of general mixing requires a multivariate/multicoordinate representation that can accommodate multiple particle species and variable surface properties, as well as the distribution of particle size. Successful extensions of moment methods to particle distribution functions characterized by more than a single mass or radius coordinate have been achieved in collaborations with Yale University for bivariate applications (Wright et al., 2001b; Rosner et al., 2003) and with our SAP partners at SUNY-SB for the fully multivariate case (Yoon and McGraw, 2003a; 2003b).

Bivariate calculations were made for the Koch-Friedlander model of nonspherical particles undergoing simultaneous coagulation and sintering (Koch and Friedlander, 1990). This well-known model provides an interesting test case for simulation of non-spherical particles of mixed size and shape (Wright et al., 2001b). Particles are characterized by two coordinates: surface area, a, and volume, v. Figure 2 shows the bivariate pdf initially (Panel a) and at a later time (Panel b) on a 150x150 grid. Sectional approaches require an unmanageable number of size bins in higher dimensions (here 22500) and just obtaining the evolved bivariate distribution shown in Panel b required about 10 calendar days on a Sun Spark Enterprise computer. (The area and volume grids in Panels a and b are logarithmically spaced and there is substantial evolution of the distribution from a to b). Moments were computed from the sectional representation and compared with the moments computed by the (bivariate) QMOM. Panels c and d of Fig. 2 show evolution of the bivariate mixed moments defined as:

$$M_{kl} = \langle v^k a^l \rangle = \int_0^\infty \int_0^\infty v^k a^l n(v,a) dv da \qquad (2.4)$$

where $n(v,a)$ is the bivariate number distribution function. QMOM calculation times ranged from several seconds (using 9 bivariate moments/ 3 quadrature points) to several minutes (using 36 bivariate moments/ 12 quadrature points) on a PC (Pentium II processor), the longer calculation requiring a nonlinear search routine to invert 36 moments to obtain the 12 quadrature points. Maximum error, relative to the sectional benchmark calculation, ranged from 1% (using 36 bivariate moments/ 12 quadrature points) to 20% (using 9 bivariate moments/ 3 quadrature points), which is quite good considering the small number of quadrature points and orders of magnitude range spanned by the moments themselves (Fig. 2). This orders-of-magnitude savings in computation time illustrates the dramatic efficiency of moment methods. It is for these kinds of problems, where the aerosol population needs to be represented by more that one coordinate, that the full advantages of the method of moments becomes evident.

The great computational efficiency of the QMOM makes this method an ideal approach for extension to fully multivariate aerosol dynamics simulations. The most significant obstacle had been the lack of a systematic and efficient means for assigning quadrature points in higher coordinate dimensions - and this has now been overcome through an extension of the QMOM using the statistical method of principal components analysis (PCA) (Yoon and McGraw, 2004a, 2004b). The idea for using PCA originated with Prof. Zhu, and AMS student Choongseok (Paul) Yoon undertook the development of this idea as part of his doctoral research project while working at BNL. In this interesting application of statistics, which might be called "dynamic PCA", the covariance matrix evolves in time as the aerosol distribution evolves. The resulting PCA-QMOM has been tested at the box model level via comparisons with results from the high-resolution bivariate (v,a) sectional model, discussed above, and compared with analytic test cases for coagulation and condensation in higher coordinate dimensions where a sectional calculation of the multivariate pdf, or indeed even visualizing this higher dimensional distribution function, is impractical (Yoon and McGraw, 2004b). Illustrative calculations from the PCA-QMOM are shown in Fig. 3 for one of the analytic test cases using three aerosol coordinates (species masses m_1, m_2, and m_3). These results are discussed further under Approach, where a proposed module designed to implement the QMOM is described. It is interesting that for all known test cases where an analytic solution for the aerosol dynamics exists, the QMOM is also exact.

In our view, the inherent complexity of aerosol processes, coupled with the need to strike a balance between model complexity and computational efficiency, will make the use of moment-based methods or some other similar statistical approach, obligatory and widespread in the future - especially for multivariate particle populations where sectional representation of the full multidimensional pdf is not an option.

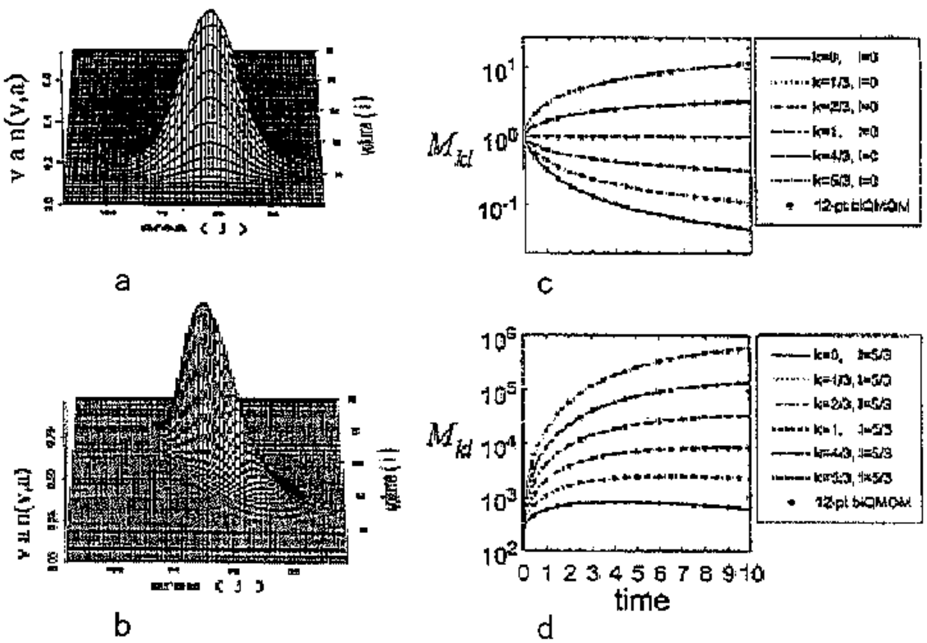

Figure 2: Evolution of a bivariate pdf under simultaneous coagulation and sintering. Panels a and b: 2D discrete model with 150x150 size sections; a. initial distribution (t =0), b. evolved distribution at t =10 with t in reduce coagulation time units. Panels c and d compare moments obtained from discrete model integration (points) with the moments evolved directly using the bivariate QMOM (curves). Results for 12 bivariate mixed moments (from Wright et al. 2001b).

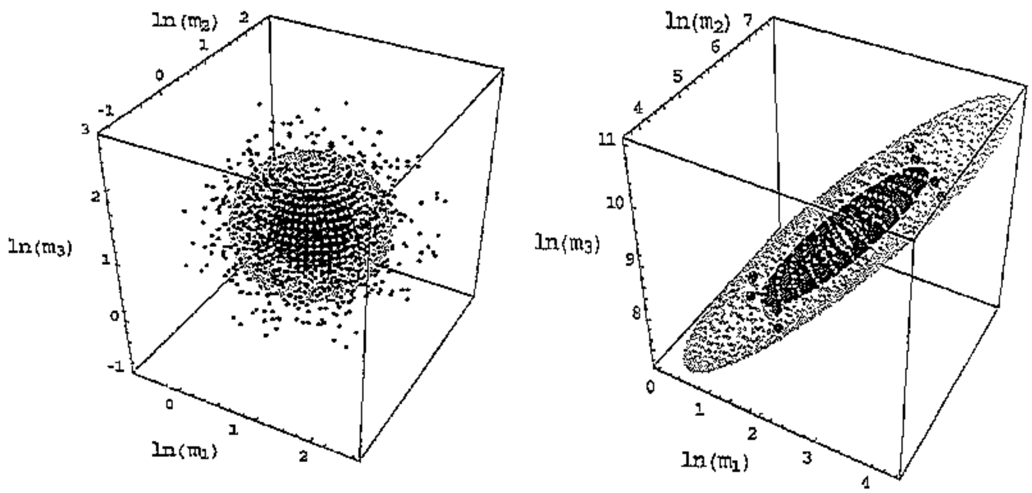

Figure 3: Evolution of a three component generally-mixed aerosol. Figure shows evolution of the σ (blue) and 2σ (green) probability surfaces under coagulation and condensation, and quadrature points (red) (from Yoon and McGraw, 2003b).

2.4.4 Parameterization of aerosol-cloud interactions

Clouds cover on average about 60% of the Earth's surface and play crucial roles in regulating the Earth's energy balance and water cycle; yet they remain the major source of uncertainty in climate models. Aerosols have major influences on clouds and through clouds on climate. First, aerosols are responsible for cloud formation, which requires the activation of aerosol particles to form cloud droplets through heterogeneous nucleation (the first indirect aerosol effect). Aerosol particles, depending on their number concentration and wetting properties, determine the cloud droplet number concentration, N_D, which in turn has a major effect on the subsequent autoconversion process whereby large cloud droplets collect smaller ones and become embryonic raindrops (second indirect aerosol effect). Meteorological conditions including temperature and concentration of water vapor also play an important role in determining number concentration through their influence on the fraction of aerosol particles that activate to become cloud droplets. Meteorological conditions also determine cloud liquid water content, L, and the cloud turbulence conditions that also play major roles in autoconversion.

Parameterizations for cloud activation vary considerably as to the level of aerosol microphysical detail that they include. The GISS GCM currently employs a mass-only aerosol representation based on multiple regression relationships used to predict cloud droplet number over land (mass concentrations of sulfate and organic matter) and over oceans (mass concentrations of sulfate, organic matter, and sea salt) (Menon et al., 2002). Other parameterizations require a higher level of size/composition detail than available in mass-only aerosol models. Examples here include parameterizations based on single or multiple lognormal, or sectional size representations of the aerosol population (Abdul-Razzak and Ghan, 2002), and recent extension of the Abdul-Razzak parameterization to include effects from particle composition and surface properties (Rissman et al., 2004). Clearly, the requirements of any aerosol-cloud parameterization to be used set a lower limit on the level of microphysical detail that the climate aerosol module must include. Recent parameterizations also include the important role played by droplet dispersion on radiative forcing (Liu and Daum, 2002). The method of moments is sufficiently flexible that it can include a variety of such parameterizations for the first indirect effect.

Parameterization of the second aerosol indirect effect has proven especially difficult (Liu and Daum, 2004). Lacking theoretical foundation, there is large discrepancy (several orders of magnitude) among existing parameterizations for the autoconversion rate. In several recent papers (McGraw and Liu, 2003; 2004; 2006) the kinetic potential (KP) of nucleation theory has been adapted to provide a new theoretical foundation for understanding drizzle formation and the second aerosol indirect effect; namely, the tendency for aerosols to increase cloud droplet number concentrations and for increased droplet number concentrations to suppress rain (Rosenfeld, 2000). The KP drizzle theory provides an explanation for a long-standing puzzle concerning the precipitation process in warm clouds (McGraw and Liu, 2004): droplets of significant fall velocity size would seem to take longer to form than the lifetime of a typical rain cloud. Drizzle in the KP description is identified as a barrier crossing process that transforms cloud droplets to drizzle size with a rate dependent on turbulent diffusion, droplet collection efficiency, and cloud droplet size (through N_D and L). The barrier regulates the rate at which cloud droplets can enter the collection regime such that those few that do enter experience less competition and can grow much more quickly to significant fall velocity size. A parameterization for the transient drizzle rate is presented in McGraw and Liu (2004).

Important to current parameterizations based on this model, the barrier maximum yields a critical droplet size, here approximately 20-30 micron in radius, having balanced condensation, collection, and evaporation rates. This newly identified critical radius provides a microphysical basis for improving Kessler-type empirical parameterizations of autoconversion rate (Liu et al., 2004; 2005; 2006), and has already been included in one parameterization employed recently in a climate model (Rotstayn and Liu, 2005).

3. Technical Approach

The technical approach is designed with two purposes in mind. First, under Task 1, we propose to develop the mathematical foundation and methods needed to expand the power, efficiency, and flexibility of new statistical approaches to aerosol simulation. Second, under Task 3, we propose to incorporate these findings into a new aerosol module designed to be compatible with the CCSM modeling framework and available for use in time for CCSM5. Parameterizations for aerosol microphysical properties and aerosol-cloud interactions are under rapid development, and becoming better rooted in physics, due in large part to DOE support through its ASP and ARM programs. Task 2 will leverage findings from several BNL programs in this area to make the newest and best parameterizations available to the climate modeling community, generally, and for use in the new aerosol module proposed under Task 3.

3.1 Task structure

3.1.1 Task 1: Developing new capabilities for aerosol simulation using advanced statistical methods and improvements to the QMOM (Years 1-3)

Multivariate statistics: A central concern of all aerosol microphysical models is how to capture the relevant aspects of particle size and composition while striking a balance between model complexity and the efficiency required for use in climate models. Thus the question emerges: What is the smallest set of variables needed to reliably represent aerosol properties in models? One cannot, and fortunately need not, answer this question for each individual particle; the answers need to be provided for the bulk of the material that contributes to the climate influence of aerosols. With these considerations in mind, we have directed much effort over the past several years to the development of statistically-based moment approaches suitable, simultaneously, for classification, model simplification (i.e. reduction in the number of aerosol internal coordinates) and rendering of the aerosol dynamics (Yoon and McGraw, 2004a; 2004b). These activities will continue with focus on the needs of the CCSM under this Task.

The results shown in Fig. 3 illustrate an early application of the statistical approach to simulation of a generally-mixed three-component aerosol evolving under simultaneous coagulation and condensation (Yoon and McGraw, 2004b). For this test an initial distribution, lognormal in each coordinate, was chosen and statistically sampled to generate the multitude of points in compositional coordinate space shown in the figure for $t = 0$. Here m_i is the mass of species i in the particle. To implement the PCA-QMOM we begin with the initial distribution, or its moments, and obtain the variances and co-variances that enter the covariance matrix, Σ. For a 3-component system this is a 3x3 symmetric matrix constructed using moments through second order. These are listed below in Eq. 3.1. Assignment of quadrature points (red points in the figure) is immediate once the eigenvalues (or principal values) of Σ have been determined. The moments themselves are updated using the quadrature points, as in the usual QMOM. These are then used to update Σ, and so on, yielding a closed system of equations for evolving the moments (Yoon and McGraw, 2004b). One advantage of the method is that it requires no a priori assumptions about the form of the size distribution to track moments. Nevertheless one is free to use distributions such as lognormal distributions consistent with the tracked moments to help visualize the pdf, or to estimate physical and optical properties of the aerosol using parameterizations where distributions are required (e.g. the cloud activation parameterization of Abdul-Razzak and Ghan (2002)), or as described in connection with Task 3, to exploit certain similarities between the QMOM and modal methods.

To gain perspective on computational burden expected from the advection of aerosol moments in a global model, consider the 10 mixed mass moments tracked during evolution of the three component generally-mixed aerosol shown in Fig. 3. These are

$$\left\{N,\langle m_1\rangle,\langle m_2\rangle,\langle m_3\rangle,\langle m_1^2\rangle,\langle m_2^2\rangle,\langle m_3^2\rangle,\langle m_1 m_2\rangle,\langle m_1 m_3\rangle,\langle m_2 m_3\rangle\right\}. \qquad (3.1)$$

N is particle number concentration, m_i is species mass, and averages are defined as in Eq. 2.4.. (The last six members of this set are the second order moments that appear in the covariance matrix.) An analogous set of 10 *spatial* moments for the distribution of an advected tracer within each 3D grid cell is carried in the Prather second-order moment advection scheme. Thus we expect similar computational burden for moment advection as in the Prather scheme. Of course this estimate does not include the computational burden required to update the mass moments within each grid box, which is where the aerosol microphysical processes come into play, but this step is known from much experience to be very fast in the computationally efficient QMOM (c.f. the fast computer times cited in connection with the *v-a* box model calculations of Sec. 2.4.3). In application of PCA to the bivariate *v-a* model only 6 moments are required, namely, any subset of moments from Eq. 3.1 that includes only two coordinates. The calculations are even faster in this case than with the 9 moment scheme described in Sec. 2.4.3 and the accuracy is about the same.

Even with this success there remains much room for improvement. Figures 2 and 3 show evolution of a single aerosol pdf. Generally, as with the multi-modal method more than one pdf is required to represent the aerosol. The main difference is that in the usual modal approximation the pdf is univariate, whereas with the PCA-QMOM it is multivariate. In either case it is important to optimize this partitioning. This is primarily a classification issue whose resolution is perhaps best achieved through the statistical analysis of measurements of aerosol composition and mixing state (described below).

Another important issue relates to certain necessary convexity conditions that any valid moments set must satisfy (Rosner et al., 2003). [Necessary and sufficient conditions for a valid moment set can be framed in terms of certain Hankel-Hadamard determinates constructed from the moments which must be positive definite (Shohat and Tamarkin, 1963)]. Generally the evolution of moments preserves validity of a moment set, however in climate models where nonlinear advection algorithms are used, correlations between moments can be broken when moments are advected as independent scalars, leading to invalid sets. One way to avoid moment failures is to implement the so-called Direct QMOM or DQMOM (Marchisio et al., 2003a; 2003b, Fox, 2003) wherein quadrature points are evolved directly during the advection step with two scalars, number and mass, assigned to each point. Other approaches are currently under development and will be considered along with the DQMOM under this Task and as part of module development (Task 3).

Composition and mixing state: Most atmospheric models assume that the aerosol is either externally or internally mixed. Each of these extreme cases can be represented using single-coordinate pdfs. Multi-modal and multi-sectional methods sample the composition space of general mixtures to some degree, but multivariate methods are required to treat the general mixing case to describe, for example, the pdfs shown in Figs. 2 and 3. Field measurements indeed support a full spectrum of mixed particle states. Aerosol mixing state determines particle optical properties (e.g. black carbon coated with sulfate), solubility, and cloud activation efficiency. Thus it is important to have a good description of generally mixed aerosols for use in climate models. The proposed research seeks to develop systematic criteria for characterization of mixing and apply these criteria to develop a compact representation of mixing state in terms of multivariate mixed moments and optimized quadrature point assignments.

As an aerosol evolves its mixing state tends to change from external to internal mixing. Insights into this evolution can be gained through inspection of the covariance matrix, Σ. Figure 3 shows the 1-σ and 2-σ probability surfaces; obtained from the eigenvalues and eigenvectors of Σ, or equivalently from the quadrature points, assuming the pdf is a trivariate lognormal distribution. The initial stages of dimensional reduction are observed as the aerosol approaches internal mixing: all particles of the same mass having nearly the same composition. This is seen in the elongation of the probability surfaces with time; revealing the emergence of a single dominant coordinate (here a function of total particle mass) that is characteristic of the approach to internal mixing under coagulation. (Initially all 3 coordinates were of equal importance). The identification of dimensional reduction is a well known application of PCA, seen here to carry over to aerosol simulations based on the PCA-QMOM. Closely related to mixing state analysis is the notion of classification that needs also to be addressed under this Task. Several approaches are next described.

Classification and optimization of aerosol representation: Our AMS partners at SUNY-SB have extensive experience in the mining and classification of large data sets (Zhu et al., 2002; Zhu et al., 2003; Wang et al., 2006). Similar algorithms are currently being applied to the analysis and classification of aerosol mass spectroscopic data in a project being developed by BNL/AMS student (Bin Xu). This Summer, we plan to utilize funding from DOE ASP to apply these methods to the data sets now being generated by several Aerodyne Aerosol Mass Spectrometers as part of the large Mexico City campaign currently in progress (March 2006). Classification and regression tree methods have been incorporated into "SpectrumMiner", which uses what we call the interactive dendogram (Imrich et al., 2002) for visualization. SpectrumMiner has been applied in preliminary studies to the classification of ambient aerosols using single-particle mass spectroscopic data collected during field campaigns in Houston and Korea (Imrich et al., 2002). Hierarchy nodes are placed on concentric circles whose radii are determined by the dissimilarity of the node's sub tree. Individual particles appear as leaf nodes along the circumference of the outer circle. Successfully larger nodes (higher-level and with more particles) appear towards the center and it is these inner branches and nodes that represent the bulk of the material that is contributing to the climate influence of aerosols. Our hypothesis is that similar classification methods can productively guide aerosol model development.

Linkages between modeling and measurement will be pursued during Year 2 and we will determine whether similar classification and regression algorithms can be used to optimize how the aerosol is represented in climate models. Specific goals will include, for example, optimization of modal (class) partitioning and quadrature-point assignment, and determining which multivariate compositional moments are best to track during the course of a climate simulation. A good example of how to proceed can be found in recent studies by Jimenez and co-workers (e.g. Zhang et al., 2005). These authors employ multivariate and factor analysis to investigate the major organic aerosol components identified in an Aerodyne Mass Spectrometer data set acquired at the EPA Pittsburgh Supersite during September 2002. Using mathematical deconvolution techniques, and a priori understanding of the organic data, two mass spectral marker peaks (at *m/z*'s 44 and 57) were selected as the first guess principal components (most likely peaks associated with CO_2^+ and $C_4H_9^+$, respectively). The reconstructed organic concentrations of hydrocarbon-like and oxygenated organic aerosols (HOA and OOA) explained 99% of the variance in the measured time series of spectra. From the standpoint of modeling guidance, the study suggest that strong consideration be given to the representation of HOA (similar to diesel exhaust, and freshly emitted traffic aerosols in urban areas), and OOA (similar to aged highly processed and oxidized organic aerosols sampled in rural areas) in atmospheric models. It is clear from this example that the measurement and modeling communities can each benefit from a cross-fertilization of ideas driven by a common need for advanced statistical methodologies similar to those we propose. Field-deployable mass- spectroscopic techniques now furnish the composition of multicomponent aerosols in real time, and in some cases on a particle-by-particle basis. The analysis of such measurements has spurred the development of sophisticated software tools for multivariate data visualization, analysis, and compression. The need for microphysically-based simulations that can be compared with these new kinds of measurements has, in turn, motivated our ideas to develop multivariate, statistically-based aerosol dynamic models – with the added benefit that these same methods are efficient enough for practical climate simulation.

3.1.2 Task 2: Parameterizations for climate models (Years 1-3)

Parameterizations are required in many components of climate modeling including aerosol dynamics and direct and indirect feedbacks. Here we describe several new parameterizations under development at BNL with support from current DOE ASP and DOE ARM science programs. These include parameterizations for new particle formation, water uptake with changes in relative humidity, sea salt aerosol production flux, and for aerosol-cloud interactions and indirect effects, including drizzle formation. Findings from these activities will be leveraged as part of Task 2 especially for use in the CCSM.

The essential output variables of the aerosol dynamics module designed under Task 1 and implement under Task 3 will be in the form of quadrature points and/or moments. These variables will be advected as scalars and passed to, for example, the aerosol optical properties and aerosol-cloud interaction parameterization modules as meteorological conditions warrant. From this multivariate information, the modules will be designed to generate various zero to two dimensional projections such as total aerosol species mass, multiple lognormal distributions (or modes) for univariate size representation along various composition coordinates, and multivariate lognormal distributions for representing more general mixing states. These are the formats required for input to the currently available cloud activation parameterizations described in Sec. 2.4.4 (see Menon et al., 2002; Abdul-Razzak and Ghan, 2002; and recent extensions of Abdul-Razzak and Ghan to include composition effects on surface tension and wetting by Rissman et al., 2004). New parameterizations that relate both the relative spectral dispersion (standard deviation of the cloud droplet distribution divided by the mean) and droplet concentration to pre-cloud aerosol properties, updraft, and turbulence parameters, will also be considered for used in the CCSM as these are developed.

Subgrid cloud processes and the indirect effects of aerosols on clouds need to be parameterized in GCMs, and parameterizations of the subgrid process have been often developed empirically and have tunable parameters. The empirical parameterizations, and especially the tunable parameters associated with them, often do not have solid theoretical bases. To improve this situation, a concerted effort has been made by BNL under its DOE

ARM program to derive parameterizations from first principles. A typical example is the development of new parameterizations for the autoconversion process (the first step for cloud droplets growing into small raindrops). Application of the new autoconversion parameterization to a GCM has produced promising results without arbitrarily tuned parameters (Rotstayn and Liu 2005). BNL will propose leveraging the best of these parameterizations for use in the CCSM in a form that makes best utilization of the moment sequences already tracked in the QMOM. Emphasis will be on aerosol-cloud interactions, especially on parameterizations of cloud turbulence, and aerosol indirect effects on droplet dispersion, cloud optical properties, and cloud lifetime.

BNL is currently developing parameterizations for atmospheric new particle formation under a DOE ASP program and will leverage these results for use in the CCSM. The new parameterization, also developed using multivariate statistical methods, will include nucleation as well as the subsequent competition between growth and coagulation loss that governs the formation of particles of climate-significant size (McGraw, 2005). BNL has also introduced a parameterization for emissions of sea salt aerosol. The new parameterization includes source terms for both particle number and particle size, with dependence on meteorological conditions, and is well suited for use in climate models (Lewis and Schwartz, 2004). BNL will also incorporate a new parameterization for the water uptake and related aerosol optical properties (Lewis, 2006). Activities under Task 2 will include leveraging these findings from DOE ASP and DOE ARM programs to insure that the resulting parameterizations are compatible with the CCSM.

3.1.3 Task 3: QMOM aerosol module development (Years 1-3)

For its proposed implementation in time for CCSM5, the QMOM will be introduced gradually, beginning with 1-pt quadrature (number and mass moments) to benefit from PNL's concurrent implementation of the modal method. The 1-pt QMOM has been tested recently and found to give accuracy comparable to the modal method (Upadhyay and Ezekoye, 2003). Multiple quadrature point methods for fully multivariate pdfs will be introduced first for the mixed mode. In this mode (MXX in Fig. 4) aerosols tend to end up with aging, so this is perhaps the most important mode, albeit the one that is the most neglected in the traditional modal and sectional approaches to aerosol dynamics. The MXX mode should provide an excellent testing ground both for studying the general mixing states of atmospheric aerosols and for development of the new statistical methods envisaged for Task 1. The new module will be thoroughly tested and benchmarked at the box-model level using high-resolution sectional and analytic methods.

	PRIMARY MODES	SECONDARY MODES	TERTIARY+ MODES
Mechanism I 14 modes 45 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, BC3, DBC, BOC, BCS	MXX
Mechanism II 14 modes 45 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, OCS, DBC, BOC, BCS	MXX
Mechanism III 11 modes 35 variables	AKK, ACC, DDD, SSA, SSC, OCC, BC1	DSS, BC2, BOC	MXX
Mechanism IV 8 modes 28 variables	ACC, DDD, SSS, OCC, BC1	DSS, BC2,	MXX

Figure 4. Modal structures developed for the NASA-GISS climate model. Primary modes: AKK = Aitken, ACC = inorganic accumulation, DDD = insoluble mineral dust, SSA = accumulation mode sea salt, SSS = total sea salt, OCC = organic carbon, BC1 = insoluble black carbon. Secondary modes are derived from the primary modes through condensation and coagulation processes. MXX = mixed mode. The user specifies which mechanism to use. (From Wright et al., 2006).

Module development will benefit from similarities between 1-pt quadrature and the modal methods (Upadhyay, R. R., and Ezekoye, O. A, 2003). Input/Output structures will be designed to be similar to those of the modal method and we envisage working with and sharing information, methods, and parameterizations with PNL investigators as findings develop - in full support of PNL's proposed implementation of the modal method as described in the inter-Laboratory proposal. BNL will also leverage findings from its current NASA program which requires building a QMOM module for the GISS GCM. The first version of the BNL module, called MATRIX (for Multiconfiguration Aerosol Tracker of mIXing state), was delivered to NASA in Feb. 06 and is currently being implemented in the GCM. An illustration of the flexibility of the multiconfiguration framework of MATRIX is shown in Fig. 4. Note that the modal structures here are somewhat subjective – as is the usual case (e.g. Jacobson, 2001; 2002). For example, DDD represents insoluble mineral dust with less than 5% sulfate coating. On further addition of sulfate, particles are transferred to the DSS soluble mineral dust mode. Such criteria are obviously somewhat arbitrary. The proposed classification methods introduced under Task 1 should provide a firmer statistical foundation to such assignments.

3.2 Tasks by individual

Robert L. McGraw, Principal Investigator (BNL). Responsible for project leadership and technical direction.

Wei Zhu, co-Principal Investigator (SUNY-SB). Responsible for many of the activities described under Task 1 and for student direction. Will lead the design of the mathematical and statistical framework for those activities described under Task 1.

Douglas Wright, co-Investigator (BNL). Contribute to the activities of Task 1 and to module development for Task 3

Yangang Liu, co-Investigator (BNL). Development of parameterizations for aerosol-cloud interaction and indirect effects under Task 2.

Ernie Lewis, co-Investigator (BNL). Development of parameterizations for aerosol water uptake (hygroscopicity) and sea salt aerosol emissions under Task 2.

3.3 Milestones

Year 1: Continue development of multivariate extensions of the QMOM. Selection of optimal moment sets for multicomponent aerosols. Development of new statistical approaches for the systematic classification of aerosol mixing states. Initiate construction of QMOM module and incorporation of microphysical parameterizations.

Year 2: Apply Visual Statistical Analyzer (ViStA) framework and similar methods, developed for classification of field aerosol measurements, to optimize modal (class) structures for aerosol simulation. Apply Bayesian statistical methods to the characterization of evolving aerosol populations. Begin benchmark validations of the QMOM aerosol module using high-resolution sectional and analytic methods.

Year 3: Completion of QMOM module validation studies. Prepare for integration into the CCSM.

4. Consortium Arrangements

The proposed statistical approaches to aerosol simulation are inherently more interesting from a mathematical perspective than either the sectional or modal methods, and require a correspondingly greater level of mathematical sophistication for their development. To effectively perform the proposed work we are building on an already successful collaboration between the BNL Atmospheric Sciences Division and the Applied Mathematics and Statistics (AMS) Department at SUNY-SB.

4.1 Why this team?

There is a strong history of productive collaboration between our groups. In recent years BNL has taken on several AMS students who have completed, or are in the late stages of completing, their doctoral research in applied mathematics while at BNL. Especially relevant to the proposed SAP is the work of Paul Yoon, an AMS student whose research was jointly supervised by Professor Zhu and Dr. McGraw. That effort has resulted in a major advancement of the multivariate QMOM for simulating the general mixing states of multicomponent aerosols. Key progress was achieved through influx of new ideas from the field of principal components analysis (PCA) (Yoon and McGraw, 2004a; 2004b). We view this as only the first breakthrough step in the application of advanced statistical methods to the science of aerosol simulation. Other statistical models such as Bayesian models, etc. will studied as part of the proposed SAP. More recently a second AMS student (Mr. Bin Xu) has been working in the BNL Atmospheric Sciences Division on visual statistical analysis and data mining methods and software. We envisage that similar statistical methods, developed initially to facilitate the analysis of atmospheric field measurements, will serve both to guide the science of aerosol simulation, for example by identifying the aerosol classes and mixing states most important to track during simulation, and help motivate new collaborations between the measurement and modeling communities.

4.2 Project management

The proposed SAP will be a partnership between BNL and SUNY-SB with BNL leading the science application work, in support of CCSM, and SUNY-SB leading the applied mathematics research. We envisage taking on perhaps two additional graduate students as part of the proposed effort. These students, as yet unidentified, would carry out their research both at SUNY-SB and BNL, and under the joint direction of Professor Zhu and BNL staff – the protocol we have used in the past. Ideally we hope to support one student from math (M) and one from computer science (CS) so as to develop a complementary set of skills for addressing the first and second of the SAP objectives, respectively, listed in Section 2.1. Students benefit from the close proximity of our two institutions, and from the combination of computational and scientific resources and staff expertise.

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OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

Statistical Approaches to Aerosol Dynamics for Climate Simulation

ORGANIZATION
Brookhaven National Laboratory

Budget Page No: 1

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR
Dr. Robert McGraw, Principal Investigator

Requested Duration: 12 (Months)
Year 1

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Man-Mo. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. McGraw, R	2	0	0		
2. Wright, D	2				
3. Liu, Y	2				
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	7	0	0	$62,779	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1			$7,739	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$70,518	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$28,912	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$99,431	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits				$3,580	
5. SUBCONTRACTS - SUNY STONY BROOK				$0	
6. OTHER - SHOP SERVICES				$0	
TOTAL OTHER DIRECT COSTS				$3,580	
H. TOTAL DIRECT COSTS (A THROUGH G)				$103,010	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus 7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus 31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden, 11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS				$86,990	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$190,000	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$190,000	

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U.S. Department of Energy

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OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

Statistical Approaches to Aerosol Dynamics for Climate Simulation

ORGANIZATION Brookhaven National Laboratory				Budget Page No: 2		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Dr. Robert McGraw, Principal Investigator				Requested Duration: 12 (Months) Year 2		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Man-Mo. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. McGraw, R	2	0	0		
2. Wright, D	2				
3. Liu. Y	2				
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	7	0	0	$65,862	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1			$8,056	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$73,918	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$30,307	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$104,225	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits				$3,752	
5. SUBCONTRACTS - SUNY STONY BROOK				$0	
6. OTHER - SHOP SERVICES				$0	
TOTAL OTHER DIRECT COSTS				$3,752	
H. TOTAL DIRECT COSTS (A THROUGH G)				$107,977	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus 7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus 31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden, 11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS				$91,392	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$199,369	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$199,369	

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U.S. Department of Energy

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OMB Control No.
1910-1400
OMB Burden Disclosure Statement on Reverse

Statistical Approaches to Aerosol Dynamics for Climate Simulation

ORGANIZATION Brookhaven National Laboratory				Budget Page No: 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR McGraw, R				Requested Duration: 12 (Months) Year 3	

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Man-Mo. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. McGraw, R	2	0	0		
2. Wright, D	2				
3. Liu, Y	2				
4.	1				
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	8	0	0	$68,497	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	1			$8,378	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$76,875	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$31,519	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$108,393	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits				$3,902	
5. SUBCONTRACTS - SUNY STONY BROOK				$0	
6. OTHER - SHOP SERVICES				$0	
TOTAL OTHER DIRECT COSTS				$3,902	
H. TOTAL DIRECT COSTS (A THROUGH G)				$112,295	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus 7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus 31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden, 11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS				$95,266	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$207,561	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$207,561	

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Budget Page

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OMB Control No.
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Statement on Reverse

Statistical Approaches to Aerosol Dynamics for Climate Simulation

ORGANIZATION: Brookhaven National Laboratory — Budget Page No: 4 - Summary

PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR: McGraw, R — Requested Duration: 36 (Months)

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Man-Mo. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. McGraw, R	7	0	0		
2. Wright, D	7				
3. Liu, Y	7				
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. (3) TOTAL SENIOR PERSONNEL (1-6)	23	0	0	$197,139	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. (1) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)	4			$24,173	
3. ( ) GRADUATE STUDENTS					
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				$221,313	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				$90,738	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				$312,049	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT				$0	
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				$0	
2. FOREIGN					
TOTAL TRAVEL				$0	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				$0	
2. TUITION & FEES				$0	
3. TRAINEE TRAVEL				$0	
4. OTHER (fully explain on justification page)				$0	
TOTAL PARTICIPANTS (0) TOTAL COST				$0	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				$0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				$0	
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES - ITD Support/Services @ 3.75% of Total Salaries + Fringe Benefits				$11,234	
5. SUBCONTRACTS - SUNY STONY BROOK				$0	
6. OTHER - SHOP SERVICES				$0	
TOTAL OTHER DIRECT COSTS				$11,234	
H. TOTAL DIRECT COSTS (A THROUGH G)				$323,283	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 39.45% General & Administrative (G&A) on Item (H) Total Direct Costs Less Item (D.) Equipment Plus 7.0% Material Burden on Item (E) Travel, Item (G.1.) Mat'ls & Supplies, Item (G.5.) Subcontracts & Item (D.) Equipment Plus 31.2% G&A Common Support on Item (G.4.) Computer Services Plus 20% Organizational Burden. 11.5% Space Charge, .35% Waste Management Fee & 2.46% Electric Power on Items A+B+C;					
TOTAL INDIRECT COSTS				$273,647	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				$596,931	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES				$0	
L. TOTAL COST OF PROJECT (J+K)				$596,931	

BNL BUDGET JUSTIFICATION

_A._ Senior Personnel: **$197,139**

The personnel costs, as budgeted, include 2.4 months per year for the Principal Investigator and 2.4 months per year for each senior personnel totaling 7.2 months per year.

All salaries in years two through three include a 4.1% COLA increase per year

_B._ Other Personnel: **$24,173**

Support for one professional include 1.2 months during year one at a rate of $7,739, 1.2 months during year two at a rate of $8,056, and 1.2 months during year three at a rate of $8,378.

_C._ Fringe Benefits: **$90,738**

This burden is calculated at the rate of 41% of total salary for regular employees.

_G._ Other Direct Costs: **$ 11,234**

Computer Services – This charge is calculated at the rate of 3.6% of Total Salaries plus Fringe Benefits and covers the annual costs for IT support services.

_H._ Total Direct Costs: **$323,283**

_I._ Indirect Costs: **$273,647**

Organizational Burden: This burden is calculated at the rate of 20% of Total Salary plus Fringe Benefits. This expense covers the costs for Departmental Management, financial and business management support services and environmental safety and health facility support services.

Space Charge: This charge is calculated at the rate of 11.5% of Total Salary plus Fringe Benefits. This expense covers the cost for the maintenance of building space and equipment.

Fuel Charge: This charge is calculated at the rate of 20.3% based on Space charge.

Waste Management Fee: This charge is calculated at the rate of .35% of Total Salary plus Fringe Benefits. This expense covers the cost for waste disposal for Environmental Sciences Department.

Electric Power: The cost for electric power is calculated at the rate of 2.46% of Total Salary plus Fringe Benefits. Note: Electric Power is exempt from BNL G&A.

BNL General and Administrative (G&A) Overhead is assessed on all BNL research activities as a percentage rate against total modified costs less electric power. G&A consists of two segments: Traditional G&A (31.20%) and Common Support G&A (8.25%).

_L._ Total Cost of Project: **$596,931**

APPLICATION FOR FEDERAL ASSISTANCE

SF 424 (R&R)

2. DATE SUBMITTED

Applicant Identifier

3. DATE RECEIVED BY STATE

State Application Identifier

1. * TYPE OF SUBMISSION

☐ Pre-application ☑ Application ☐ Changed/Corrected Application

4. Federal Identifier

5. APPLICANT INFORMATION * Organizational DUNS: 8048782470000

* Legal Name: Research Foundation of SUNY

Department: Office of Sponsored Programs Division:

* Street1: SUNY at Stony Brook Street2:

* City: Stony Brook County: Suffolk * State: NY * ZIP Code: 11794-3362

* Country: USA

Person to be contacted on matters involving this application

Prefix:	* First Name:	Middle Name:	* Last Name:	Suffix:
Ms.	Laureen		Velez	

* Phone Number: 631-632-4402 Fax Number: 631-632-6963 Email: lvelez@notes.cc.sunysb.eud

6. * EMPLOYER IDENTIFICATION *(EIN) or (TIN):* 14-1368361

7. * TYPE OF APPLICANT: P: Other (specify)

Other (Specify): Private Not for Profit

Small Business Organization Type

☐ Women Owned ☐ Socially and Economically Disadvantaged

8. * TYPE OF APPLICATION: ☑ New

☐ Resubmission ☐ Renewal ☐ Continuation ☐ Revision

If Revision, mark appropriate box(es).

☐ A. Increase Award ☐ B. Decrease Award ☐ C. Increase Duration

☐ D. Decrease Duration ☐ E. Other *(specify)*:

* Is this application being submitted to other agencies? Yes ☐ No ☑

What other Agencies?

9. * NAME OF FEDERAL AGENCY: Chicago Service Center

10. CATALOG OF FEDERAL DOMESTIC ASSISTANCE NUMBER: 81.049

TITLE: Office of Science Financial Assistance Program

11. * DESCRIPTIVE TITLE OF APPLICANT'S PROJECT:

Statistical Approaches to Aerosol Dynamics for Climate Simulation

12. * AREAS AFFECTED BY PROJECT *(cities, counties, states, etc.)*

National

13. PROPOSED PROJECT:

* Start Date: 07/01/2006 * Ending Date: 06/30/2009

14. CONGRESSIONAL DISTRICTS OF:

a. * Applicant: NY 01 b. * Project: NY 01

15. PROJECT DIRECTOR/PRINCIPAL INVESTIGATOR CONTACT INFORMATION

Prefix:	* First Name:	Middle Name:	* Last Name:	Suffix:
Dr.	Wei		Zhu	

Position/Title: Professor * Organization Name: SUNY at Stony Brook

Department: Dept. of Applied Math & Statis Division:

* Street1: SUNY at Stony Brook Street2:

* City: Stony Brook County: Suffolk * State: NY * ZIP Code: 11794-3600

* Country: USA

* Phone Number: 631-632-8374 Fax Number: 631-632-8490 * Email: zhu@ams.sunysb.edu

OMB Number: 4040-0001

Expiration Date: 04/30/2008

SF 424 (R&R) APPLICATION FOR FEDERAL ASSISTANCE

16. ESTIMATED PROJECT FUNDING

a. * Total Estimated Project Funding	382,513.00
b. * Total Federal & Non-Federal Funds	382,513.00
c. * Estimated Program Income	0.00

17. * IS APPLICATION SUBJECT TO REVIEW BY STATE EXECUTIVE ORDER 12372 PROCESS?

a. YES ☐ THIS PREAPPLICATION/APPLICATION WAS MADE AVAILABLE TO THE STATE EXECUTIVE ORDER 12372 PROCESS FOR REVIEW ON:

DATE:

b. NO ☐ PROGRAM IS NOT COVERED BY E.O. 12372; OR

☑ PROGRAM HAS NOT BEEN SELECTED BY STATE FOR REVIEW

18. By signing this application, I certify (1) to the statements contained in the list of certifications* and (2) that the statements herein are true, complete and accurate to the best of my knowledge. I also provide the required assurances * and agree to comply with any resulting terms if I accept an award. I am aware that any false, fictitious, or fraudulent statements or claims may subject me to criminal, civil, or administrative penalties. (U.S. Code, Title 18, Section 1001)

☐ * I agree

** The list of certifications and assurances, or an internet site where you may obtain this list, is contained in the announcement or agency specific instructions.*

19. Authorized Representative

Prefix:	* First Name:	Middle Name:	* Last Name:	Suffix:
Ms.	Lydia		Chabza	

* Position/Title: Sponsored Programs Administrator
* Organization: Research Foundation of SUNY
Department: Office of Sponsored Programs
Division:
* Street1: SUNY at Stony Brook
Street2:
* City: Stony Brook
County: Suffolk
* State: NY
* ZIP Code: 11794-3362
* Country: USA
* Phone Number: 631-632-4402
Fax Number: 631-632-6963
* Email: lchabza@notes.cc.sunysb.edu

* Signature of Authorized Representative	* Date Signed
Completed on submission to Grants.gov	Completed on submission to Grants.gov

20. Pre-application [Add Attachment] [Delete Attachment] [View Attachment]

OMB Number: 4040-0001
Expiration Date: 04/30/2008

DOE F 4620.1
(04-93)
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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No. 1910-1400
OMB Burden Disclosure Statement on Reverse

ORGANIZATION RESEARCH FOUNDATION OF SUNY				Budget Page No: 1		
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Wei Zhu				Requested Duration: 12 (Months)		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested by Applicant	Funds Granted by DOE	
	CAL	ACAD	SUMR			
1. Wei Zhu, PI			3.00	27,381.00		
2.						
3.						
4.						
5.						
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)						
7. ( ) TOTAL SENIOR PERSONNEL (1-6)				27,381.00	0.00	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( ) POST DOCTORAL ASSOCIATES						
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)						
3. (2) GRADUATE STUDENTS				39,840.00		
4. ( ) UNDERGRADUATE STUDENTS						
5. ( ) SECRETARIAL - CLERICAL						
6. ( ) OTHER						
TOTAL SALARIES AND WAGES (A+B)				67,221.00	0.00	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				9,025.00		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				76,246.00	0.00	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)						
TOTAL PERMANENT EQUIPMENT						
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)						
2. FOREIGN						
TOTAL TRAVEL				0.00	0.00	
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)						
2. TUITION & FEES						
3. TRAINEE TRAVEL						
4. OTHER (fully explain on justification page)						
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00	
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER (ADPE) SERVICES						
5. SUBCONTRACTS						
6. OTHER				6,912.00		
TOTAL OTHER DIRECT COSTS				6,912.00	0.00	
H. TOTAL DIRECT COSTS (A THROUGH G)				83,158.00	0.00	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 55% of A, B and C						
TOTAL INDIRECT COSTS				41,935.00		
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				125,093.00	0.00	
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES						
L. TOTAL COST OF PROJECT (J+K)				125,093.00	0.00	

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Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION RESEARCH FOUNDATION OF SUNY				Budget Page No: 2	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Wei Zhu				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Wei Zhu, PI			3.00	28,202.00	
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)				28,202.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				39,840.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				68,042.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				9,749.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				77,791.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				6,912.00	
TOTAL OTHER DIRECT COSTS				6,912.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				84,703.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 55% of A, B, and C					
TOTAL INDIRECT COSTS				42,785.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				127,488.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				127,488.00	0.00

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U.S. Department of Energy
Budget Page
(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION RESEARCH FOUNDATION OF SUNY				Budget Page No: 3	
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Wei Zhu				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos.			Funds Requested	Funds Granted
	CAL	ACAD	SUMR	by Applicant	by DOE
1. Wei Zhu, PI			3.00	29,049.00	
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)				29,049.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				39,840.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				68,889.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				10,479.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				79,368.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				6,912.00	
TOTAL OTHER DIRECT COSTS				6,912.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				86,280.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 55% of A, B and C					
TOTAL INDIRECT COSTS				43,652.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				129,932.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				129,932.00	0.00

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Budget Page

(See reverse for Instructions)

OMB Control No.
1910-1400
OMB Burden Disclosure
Statement on Reverse

ORGANIZATION RESEARCH FOUNDATION OF SUNY				Budget Page No:	4
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR Wei Zhu				Requested Duration:	CUMULATIVE (Months)
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)	DOE Funded Person-mos. CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Wei Zhu, PI			9.00	84,632.00	
2.					
3.					
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)					
7. ( ) TOTAL SENIOR PERSONNEL (1-6)				84,632.00	0.00
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. ( ) POST DOCTORAL ASSOCIATES					
2. ( ) OTHER PROFESSIONAL (TECHNICIAN, PROGRAMMER, ETC.)					
3. (2) GRADUATE STUDENTS				119,520.00	
4. ( ) UNDERGRADUATE STUDENTS					
5. ( ) SECRETARIAL - CLERICAL					
6. ( ) OTHER					
TOTAL SALARIES AND WAGES (A+B)				204,152.00	0.00
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				29,253.00	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				233,405.00	0.00
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM.)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN					
TOTAL TRAVEL				0.00	0.00
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)					
2. TUITION & FEES					
3. TRAINEE TRAVEL					
4. OTHER (fully explain on justification page)					
TOTAL PARTICIPANTS ( ) TOTAL COST				0.00	0.00
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES					
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION					
3. CONSULTANT SERVICES					
4. COMPUTER (ADPE) SERVICES					
5. SUBCONTRACTS					
6. OTHER				20,736.00	
TOTAL OTHER DIRECT COSTS				20,736.00	0.00
H. TOTAL DIRECT COSTS (A THROUGH G)				254,141.00	0.00
I. INDIRECT COSTS (SPECIFY RATE AND BASE) 55% of A, B and C					
TOTAL INDIRECT COSTS				128,372.00	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				382,513.00	0.00
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES					
L. TOTAL COST OF PROJECT (J+K)				382,513.00	0.00

BUDGET JUSTIFICATION

SECTION

A. Senior Personnel **$ 97,750**

The personnel costs, as budgeted, include three summer months per year for the Principal Investigator. Faculty monthly summer salaries are budgeted at 1/9 of academic year salary.

SUNY Research Foundation fringe benefit rate is calculated at 15.5% each year.

All salaries in years two through three include a three percent COLA increase per year.

B. Other Personnel **$ 135,655**

Support for two graduate students during the calendar year at a rate of $19,920 per year per student.

SUNY Research Foundation fringe benefit rates are calculated as follows:

	Year 1	Year 2	Year 3
Graduate Students	12.0%	13.5%	15.0%

Salaries and wages are competitive with those of other public and private research universities of similar research standing to Stony Brook.

F. Other Direct Costs **$ 20,736**

Graduate Student Tuition costs are included for the two graduate students at six credits per year calculated at the current New York State resident rate of $3,456.

G. Total Direct Costs **$ 254,141**

H. Indirect Costs **$ 128,372**

Indirect costs are calculated on all direct costs, except tuition, at a rate of 55.0%.

I. Total Cost of Project **$ 382,513**

CURRENT AND PENDING SUPPORT

Robert McGraw

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
BNL	Developing new theory and parameterizations for clouds and precipitation in climate models (Principal Investigator)	Active	DOE ARM	10/1/2005-9/30/2008	$120K	0.2FTE
BNL	New particle formation: Mechanisms and influence on atmospheric aerosol properties (Principal Investigator)	Active	DOE ASP	10/1/2005-9/30/2008	$113K	0.4
BNL	Development of Aerosol and Cloud Microphysics Schemes for the GISS Climate Model (Principal Investigator)	Active	NASA	2/1/2006-1/31/2008	$110K	0.1
BNL	Aerosol Cloud Interactions: Field Studies and Interpretation (co-Investigator)	Active	DOE ARM	10/1/2005-9/30/2008	$600K	0.05
BNL	Modeling Aerosol Processes in the DOE Atmospheric Science Program (co-Investigator)	Active	DOE ASP	10/1/2005-9/30/2008	$450K	0.05
BNL	Statistical approaches to aerosol dynamics for climate simulation (Principal Investigator)	Pending (SAP for this proposal)	DOE SciDAC2	7/1/2006-6/30/2009	$315K	0.2

Douglas L. Wright Jr

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
BNL	Development of an Observation-Based Photochemical-Aerosol Modeling System (Principal Investigator)	Active	BNL (LDRD)	10/1/04-9/30/06	$72K	0.3FTE
BNL	Development of Aerosol and Cloud Microphysics Schemes for the GISS Climate Model (co-Investigator)	Active	NASA	2/1/2006-1/31/2008	$110K	0.2
BNL	Modeling Aerosol Processes in the DOE Atmospheric Science Program (co-Investigator)	Active	DOE ASP	10/1/2005-9/30/2008	$450K	0.5
BNL	Statistical approaches to aerosol dynamics for climate simulation (co-Investigator)	Pending (SAP for this proposal)	DOE SciDAC2	7/1/2006-6/30/2009	$315K	0.2

Yangang Liu

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
BNL	Developing new theory and parameterizations for clouds and precipitation in climate models (co-PI)	Active	DOE ARM	10/1/2005-9/30/2008	$120K	0.2FTE
BNL	Aerosol Cloud Interactions: Field Studies and Interpretation (co-PI)	Active	DOE ARM	10/1/2005-9/30/2008	$600K	0.3
BNL	Parameterizations of Cloud Microphysics and Indirect Aerosol Effects (co-PI)	Active	DOE ARM	10/1/2006-9/30/2008	$2200K	0.3
BNL	Statistical approaches to aerosol dynamics for climate simulation (co-PI)	Pending (SAP for this proposal)	DOE SciDAC2	7/1/2006-6/30/2009	$315K	0.2

Ernie Lewis

Institution	Name	Active or Pending	Funding Agency or Org.	Inclusive Dates of Project	Annual funding	Level of Effort
BNL	Shortwave radiative forcing by tropospheric aerosols (co-Investigator)	Active	DOE ARM	10/1/2005-9/30/2008	$250K	0.9FTE
BNL	Statistical approaches to aerosol dynamics for climate simulation (co-Investigator)	Pending (SAP for this proposal)	DOE SciDAC2	7/1/2006-6/30/2009	$315K	0.1

Current and Pending Support: Wei Zhu

Project/Proposal Title: Correlational Analysis of SAGE and Gene Microarray Data
Support: Current
PI: W. Zhu
Source of Support: Foster Foundation
Award Amount: $100,000
Period Covered: 02/01/04-12/31/06
Location of Project: SUNY at Stony Brook
Person-Months (or percentage) Committed to Project: 0.5 month/year

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Project/Proposal Title: The Mass-Spectra Classification Engine
Support: Current
PI: W. Zhu
Source of Support: Brookhaven National Laboratory (BNL)
Award Amount: $150,000
Period Covered: 10/01/01-12/31/06
Location of Project: BNL
Person-Months (or percentage) Committed to Project: 0.0 month/year

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Project/Proposal Title: Brain Functional Connectivity Analysis Using PET Data
Support: Current
PI: W. Zhu
Source of Support: BNL
Award Amount: $60,000
Period Covered: 09/01/04-08/31/06
Location of Project: BNL
Person-Months (or percentage) Committed to Project: 0.0 month/year

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Project/Proposal Title: Sampling Statistics and Economics of the Newly Emerging Soil Analytical Modalities
Support: Current
PI: W. Zhu
Source of Support: BNL
Award Amount: $60,000
Period Covered: 01/01/06-12/31/07
Location of Project: BNL
Person-Months (or percentage) Committed to Project: 0.0 month/year

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Project/Proposal Title: GCRC SBU with Imaging Facility at BNL
Support: Current
PI: N. Edelman
Source of Support: NIH
Award Amount: $1,700,000
Period Covered: 12/01/03-11/30/06
Location of Project: SUNY at Stony Brook and BNL

Person-Months (or percentage) Committed to Project: 3.0 months/year

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Project/Proposal Title: The Alzheimer's Disease Center Grant
Support: Current
PI: S. Ferris
Co-PI: M. de Leon, B. Reisberg, T. Wisniewski, M. Mittelman, W. Zhu
Source of Support: NIH
Award Amount: $1,000,000
Period Covered: 05/01/05-04/30/10
Location of Project: NYU
Person-Months (or percentage) Committed to Project: 2.0 months/year

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Project/Proposal Title: Cost Effective Designs for Practitioners
Support: Current
PI: W. Wong
Co-PI: H. Dette, W. Zhu
Source of Support: NIH
Award Amount: $800,000
Period Covered: 09/01/05-08/31/08
Location of Project: UCLA and SUNY Stony Brook, USA; Ruhr-Universität Bochum, Germany
Person-Months (or percentage) Committed to Project: 2.0 months/year

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Project/Proposal Title: A Unified Gene-Protein Analysis Platform at the Systems Biological Level
Support: Pending
PI: W. Zhu
Source of Support: DOE
Award Amount: $654,309
Period Covered: 07/01/06-06/30/09
Location of Project: SUNY at Stony Brook and BNL
Person-Months (or percentage) Committed to Project: 1.6 months/year

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Project/Proposal Title: Statistical Approaches to Aerosol Dynamics for Climate Simulation
Support: Pending
PI: R. McGraw
Co-PI: W. Zhu
Source of Support: DOE
Award Amount: $382,514
Period Covered: 07/01/06-06/30/09
Location of Project: SUNY at Stony Brook and BNL
Person-Months (or percentage) Committed to Project: 3.0 months/year

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(* Note: W. Zhu will reduce her effort on the NIH supported project "GCRC SBU with Imaging Facility at BNL, PI. N. Edelman" if the SciDAC proposals are funded.)

Biographical Sketches

Robert L. McGraw
Atmospheric Sciences Division
Brookhaven National Laboratory
Upton, NY 11973
Tel: 631-344-3086
Fax: 631-344-2887
e-mail: rlm@bnl.gov
SS: 155-42-0985

EDUCATION

1979 Ph.D. Physical Chemistry, University of Chicago.
1974 M.S. Chemistry, University of Chicago.
1972 B.S. Chemistry, Drexel University, Philadelphia, PA

EMPLOYMENT

2005 -	Deputy Division Head, Atmospheric Sciences Division, Brookhaven National Laboratory
2003 -	Senior Scientist, Brookhaven National Laboratory
1998 -2003	Member Brookhaven Council (Council Secretary 2001-2003)
1993 -2003	Scientist, Brookhaven National Laboratory (Tenured from 1995)
1985 -1993	Member Technical Staff, Rockwell International Science Center, Thousand Oaks, CA
1990 –1993	Member Scientific Advisory Board, Rockwell International North American Aircraft Division (now part of Boeing)
1983 -1985	Associate Scientist, Brookhaven National Laboratory
1981 -1983	Assistant Scientist, Brookhaven National Laboratory
1977 -1981	Postdoctoral Research Associate, Chemistry Department, University of California Los Angeles

RESEARCH ACTIVITIES/INTERESTS

Atmospheric aerosol microphysics and simulation methods; Homogeneous and heterogeneous nucleation of supercooled vapors and vapor mixtures as mechanisms for gas-to-particle conversion; Cloud microphysics and precipitation; Nucleation in condensed phase systems; Statistical physics and computational modeling of light propagation and scattering in materials for nonlinear optics applications.

JOURNAL PUBLICATIONS (10 out of 95 shown)

Five Recent Publications

McGraw, R., and Liu, Y. (2006), Brownian drift-diffusion model for evolution of droplet size distributions in turbulent clouds, Geophys. Res. Lett., 33, L03802, doi:10.1029/2005GL023545.

Liu, Y., Daum, P. H., McGraw, R., and Wood R. (2006), Parameterization of the autoconversion process. Part II: Generalization of Sundqvist-type parameterizations, J. Atmos. Sci., in press.

Liu, Y., Daum, P. H. and McGraw, R. (2005), Size truncation effect, threshold behavior, and a new type of autoconversion parameterization, Geophysical Research Letters, 32, L11811, doi:10.1029/2005GL022636.

Yoon, C., and McGraw, R. (2004) Representation of generally-mixed multivariate aerosols by the quadrature method of moments: I. Statistical foundation. J. Aerosol Sci. 35, 561-576 (2004).

Yoon, C., and McGraw, R., (2004) Representation of generally-mixed multivariate aerosols by the quadrature method of moments. II Aerosol dynamics, J. Aerosol Sci. 35, 577-598 (2004).

Five Other Publications

McGraw, R. and Liu, Y. (2004), Analytic formulation and parameterization of the kinetic potential theory for drizzle formation, Phys. Rev. E 70, 031606.

Liu, Y., Daum, P. H., and McGraw, R. (2004), An analytic expression for predicting the critical radius in the autoconversion parameterization, Geophys. Res. Letts. 31, L06121, doi: 10.1029/2003GL019117.

McGraw, R. and Wright, D. L. (2003), Chemically-resolved aerosol dynamics for internal mixtures by the quadrature method of moments. J. Aerosol Sci. 34, 189-209.

McGraw, R., and Liu, Y. (2003) Kinetic potential and barrier crossing: A model for warm cloud drizzle formation, Phys. Rev. Letts. 90, paper 018501, 1-4 (2003).

McGraw, R. and D. Wu (2003), Kinetic extensions of the nucleation theorem. J. Chem. Phys., 118, 9337-9347.

SYNERGISTIC ACTIVITIES

Appointed Professor Adjunct at Yale University (July 1, 2005). Instructor for Yale Grad School Fall '05 Course "Nucleation Theory" in the Chemical Engineering Department. Led development of aerosol nucleation and growth models based on the method of moments. Developed aerosols modules incorporated into several prominent atmospheric chemical transport models including GChM-O (a hemispheric scale model), and MAQSIP (a regional scale model). A new aerosol module based on the quadrature method of moments will be implemented this year in the NASA GISS climate model.

Aerosol nucleation and growth processes modules have been incorporated into 3D Eulerian plume models under DOE/NN20 support. In an earlier collaboration with INEEL, a preliminary version of our aerosol module was used for the simulation of nucleation and growth processes in a plasma quench reactor designed for nanoparticle generation.

COLLABORATORS

M. Kulmala (U. of Helsinki)
A. Laaksonen (U. of Kuopio)
R. LaViolette
P. Mirabel (U. Louis Pasteur, Strasbourg)
H. Reiss (UCLA)
D. Rosner (Yale)
S. Schwartz (Brookhaven National Lab)
J. Seinfeld (Caltech)
H. Vehkamaki (U. of Helsinki)
R. Weber (Georgia Tech.)
D. Wu (Yale)
D. Koch (NASA GISS)
S. Bauer (NASA GISS)

OTHER AFFILIATIONS

Yale University (Professor Adjunct)

Graduate Students and Post-Doctoral Scholars Sponsored

Douglas Wright, Former Post Doc
Paul Yoon, Grad. PhD Student (Applied Mathematics/Statistics)
Bin Xu, Grad. PhD Student (Applied Mathematics/Statistics)

Graduate and Post-Doctoral Advisors

Stuart A. Rice; Graduate Advisor
Howard Reiss; Post-Doctoral Advisor

Douglas L. Wright Jr. (Associate Physicist)
Atmospheric Sciences Division
Brookhaven National Laboratory
Upton, NY 11973
Tel: 631-344-3829
Fax: 631-344-2887
e-mail: dwright@bnl.gov

EDUCATION

1993 Ph.D. Chemical Physics, Virginia Commonwealth University
1987 B.A. Philosophy, Virginia Commonwealth University

PROFESSIONAL EXPERIENCE

Virginia Commonwealth University: Department of Physics, Faculty, 2003-2004
Virginia Commonwealth University: Department of Chemistry, 1993-1997, 2003-2004

Brookhaven National Laboratory	
Atmospheric Sciences Division :	(2004-present, Associate Physicist)
	(1998-1999, Contracter/Postdoctoral Fellow)
Duke University:	(2000-2001, Postdoctoral Fellow)

SELECTED PUBLICATIONS

D. Wright, Shaocai Yu, P. S. Kasibhatla, R. McGraw, S. E. Schwartz, V. K. Saxena and G.K. Yue, Retrieval of aerosol properties from moments of the particle size distribution for kernels involving the step function, J. Aerosol Sci., 33, 319, 2002.

D. Wright, P. S. Kasibhatla, R. McGraw and S. E. Schwartz, Description and evaluation of a six-moment aerosol microphysical module for use in atmospheric chemical transport models, J. Geophys. Res. 106, 20275, 2001.

D. Wright, R. McGraw and D. E. Rosner, Bivariate extension of the quadrature method of moments for modeling simultaneous coagulation and particle restructuring in flames, J. Colloid and Interface Sci. 236, 242, 2001.

D. Wright, R. McGraw, C. M. Benkovitz and S. E. Schwartz, Six-moment representation of multiple aerosol populations in a subhemipheric chemical transformation model, Geophys. Res. Lett. 27, 967, 2000.

D. Wright, Retrieval of optical properties of atmospheric aerosols from moments of the particle size distribution, J. Aerosol Sci. 31, 1, 2000.

YANGANG LIU (Associate Scientist BNL; Associate Chief Scientist for DOE ARM Program)
lyg@bnl.gov

EDUCATION

Desert Research Institute, University and Community College System of Nevada (Ph.D., Atmospheric Sciences, 1998); Nanjing Institute of Meteorology, China (B.S., Atmospheric Sciences,1983; M.S., 1989);

RESEARCH INTERESTS

Aerosol/cloud physics; light scattering and radiation transfer; remote sensing of particle properties; climate and climate change (esp., aerosol-cloud-dynamics-radiation-climate interactions); computer simulations; inverse problems.

PROFESSIONAL AFFILIATIONS

American Association for the Advancement of Science; Society for Industrial and Applied Mathematics; American Meteorological Society; American Geophysical Union

Summary of Experiences

Scientist, Chinese Academy of Meteorological Sciences, 1989-93; Research/Teaching Assistant, Desert Research Institute, University of Nevada-Reno, 1993-98; Research Associate, Brookhaven National Laboratory, 1998 to 2001; Assistant Scientist, Brookhaven National Laboratory 2001 to 2003; Associate Scientist, Brookhaven National Laboratory 2003 to present.

SELECTED Peer-Reviewed PUBLICATIONS (8 out of 42)

Liu, Y., P. H. Daum, P. H., and S. Yum (2006) , Analytical expression for the relative dispersion of the cloud droplet size distribution. Geophys. Res. Lett., 33, L02810, doi:10.1029/2005GL024052

McGraw, R., and Liu, Y. (2006), Brownian drift-diffusion model for evolution of droplet size distributions in turbulent clouds, Geophys. Res. Lett., 33, L03802, doi:10.1029/2005GL023545.

Liu, Y., Daum, P. H., McGraw, R., and Wood R. (2006), Parameterization of the autoconversion process. Part II: Generalization of Sundqvist-type parameterizations, J. Atmos. Sci., in press.

Liu, Y., Daum, P. H. and McGraw, R. (2005), Size truncation effect, threshold behavior, and a new type of autoconversion parameterization, Geophys. Res. Lett, 32, L11811, doi:10.1029/2005GL022636.

Rotstayn, L. D. and Liu,Y (2005), A smaller global estimate of the second indirect aerosol effect. Geophys. Res. Lett. 32, L05708, 10.1029/2004GL021922.

Liu, Y., Daum, P. H., and McGraw, R., (2004), An analytical expression for predicting the critical radius in the autoconversion parameterization. Geophys. Res. Lett. 31, L06121, 10.1029/2003GL019117.

Liu, Y. and Daum, P. H. (2004), Parameterization of the autoconversion process. Part I: Analytical formulation of the Kessler-type parameterizations. J. Atmos. Sci., 61, 1539-1548..

Rotstayn, L. D. and Liu, Y., (2003), Sensitivity of the indirect aerosol effect to an increase of cloud droplet spectral dispersion with droplet number concentration. J. Climate 16, 3476-3481.

Liu, Y. and Daum, P. H. Indirect warming effect from dispersion forcing. Nature 419, 580-581 (2002).

Ernie R. Lewis, Environmental Science Associate I
Atmospheric Sciences Division
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631-344-2887 (fax)
elewis@bnl.gov

EDUCATION

1990 A.B.D., Physics, University of Texas at Austin, Austin, Texas
1982 Diploma, Fluid Mechanics, von Karman Institute for Fluid Dynamics, Brussels, Belgium
1979 B.S. (honors), Physics, California Institute of Technology, Pasadena, California

EMPLOYMENT

1998- Atmospheric Sciences Division, Brookhaven National Laboratory
1994-1998 Department of Oceanography, Brookhaven National Laboratory
1980-1981 Noise Research Division, Boeing Aircraft Corporation

RESEARCH ACTIVITIES/INTERESTS

Light scattering and radiative transport in the atmosphere and aerosol-radiative interactions.
Hygroscopic and thermodynamic properties of aerosol particles and the effects of relative humidity on their chemical and physical properties.
Sea salt aerosols and their properties, concentrations, and production.
Studies in the atmospheric environment pertaining to global warming.
Climate and climate change, and the effect of aerosols on climate change.
The carbon dioxide system in the oceans.
Measurement of chemical and physical properties of seawater.
Air-sea exchange of gases and particles.

SELECTED PUBLICATIONS

Lewis, E. R., The Effect of Surface Tension (Kelvin Effect) on the Equilibrium Radius of a Hygroscopic Aqueous Aerosol Particle, submitted to *Journal of Aerosol Science*, 2006.

Lewis E. R. and Schwartz S. E., Comment on "Size distribution of sea-salt emissions as a function of relative humidity" *Atmos. Environ.* 40, 588-590 (2006); doi:10.1016/j.atmosenv.2005.08.043

Lewis E. R. and Schwartz S. E., *Sea Salt Aerosol Production: Mechanisms, Methods, Measurements, and Models – A Critical Review.* Geophysical Monograph Series Vol. 152, (American Geophysical Union, Washington, 2004).

Lewis, E., and D. W. R. Wallace. 1998. *Program Developed for CO2 System Calculations.* ORNL/CDIAC-105. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee.

Vita: Wei Zhu

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Professional Preparation

East China Normal University, Mathematics, BS, 1989
University of Illinois at Chicago, Statistics, MS, 1992
University of California Los Angeles, Biostatistics, Ph.D. 1996

Appointments

2003-	Adjunct Associate Professor, New York University
2003-	Associate Professor, SUNY at Stony Brook
1997-2003	Assistant Professor, SUNY at Stony Brook
1996-1997	Visiting Assistant Professor, SUNY at Stony Brook

Honors: Forty under 40, Long Island Business News (2004);
Promising Inventor Award, SUNY Research Foundation (2003).

Selected Recent Publications:

1. Zhu, W., Wang, X., Kovach, J. (2002). Comprehensive Statistical Spectrum Analysis Routine - Algorithm for Proteomics Analysis. Patent application through the State University of New York.
2. Zhu, W., Wang, X., Ma, Y., Rao, M.L., Glimm, J. and Kovach, J. [2003]. Detection of Cancer Specific Markers Amidst Massive Mass Spectral Data. *Proceedings of the National Academy of Sciences*. **100(25)**, 14666-14671.
3. Zhu, W., Volkow, N.D., Ma, Y., Fowler, J.S., and Wang, G-J. [2004]. Relationships of Ethanol Induced Changes in Brain Regional Metabolism and Motor, Behavioral and Cognitive Functions. *Alcohol and Alcoholism*. **39(1)**, 53-58.
4. Joo, J., Ahn, H., Lombardo, F., Hadjiargyrou, M., and Zhu, W. [2004]. Statistical Approaches in the Analysis of Gene Expression Data Derived from Bone Regeneration Specific cDNA Microarrays. *Journal of Biopharmaceutical Statistics*. **14**, 607-628.
5. Mugno, R., Zhu, W., and Rosenberger, W. [2004]. Adaptive Urn Designs for Estimating Several Percentiles of a Dose-Response Curve. *Statistics in Medicine*. **23(13)**, 2137-50.
6. Dette, H., Wong, W.K., and Zhu, W. [2005]. On the Equivalence of Optimality Design Criteria for the Placebo-Treatment Problem. *Statistics and Probability Letters*. In press.
7. Biedermann, S., Dette, H., and Zhu, W. Compound Optimal Designs for Percentile Estimation in Dose-Response Models with Restricted Design Intervals. *Journal of Statistical Planning and Inference*. To appear.
8. Biedermann, S., Dette, H., and Zhu, W. Optimal Designs for Dose-Response Models with Restricted Design Spaces. *Journal of the American Statistical Association*. To appear.
9. Wang, X, Zhu, W., Pradhan, K., Ji, C., Ma, Y., Semmes, O.J., Glimm, J and Mitchell, J. Feature Extraction in the Analysis of Proteomic Mass Spectra. *Proteomics*. To appear.
10. Km J, Zhu W, Chang L, Benter P, Ernst T. A Unified Structural Equation Modeling Approach for the Analysis of Multi-Subject, Multivariate Functional MRI Data. *Human Brain Mapping*. To appear.

SBU FACILITIES AND RESOURCES

The Department of Applied Mathematics and Statistics at the State University of New York at Stony Brook (SBU), has a network of approximately 40 UNIX work stations and 120 PC's. The Department also has a 200-node super computer, the AMS Galaxy, for intensive parallel computing.

There are approximately 200 square feet office space available in the secure computer room which contains the AMS super computer, Galaxy, at the Department of Applied Mathematics and Statistics, SUNY Stony Brook. It will host the computer equipments in supporting of this project.

Currently we have 6 UNIX stations and 15 PC work stations available to host the proposed software development. We also have access to the 200-node AMS Galaxy.

Appendix: SUNY Stony Brook Milestones and Deliverables

Our previous collaborations with BNL has achieved (1) major advances of aerosol moment methods through a novel application of principal components analysis and through the use of quadrature, both for closure of the moment evolution equations and for estimation of aerosol physical and optical properties directly from moments [see papers with AMS student C. Yoon listed under the McGraw biosketch heading of recent publications]. Joint with our BNL colleagues, we have also (2) led the development of advanced aerosol classification and time series analysis methods and software.

In this proposal, SUNY-Stony Brook will lead the mathematical development of (1) new capabilities for aerosol simulation using advanced statistical methods and improvements to the quadrature method of moments (QMOM), and (2) new capabilities for aerosol classification and time series analysis methods. In addition, (3) we will compile the necessary computer code for the newly developed methods. Our task break- down by funding years is as follows.

Year 1.
Task 1. Compile the necessary code to integrate the multivariate QMOM method developed during our previous collaborations into the SAP/SA software deliverable.

Task 2. Start the mathematical development of new capabilities to the multivariate QMOM, especially the optimized modal (class) partitioning, quadrature point assignment, and to determine which multivariate compositional moments are best to track during the course of a simulation.

Year 2.
Task 1. Aim to finish the major theoretical evaluations and derivations of new mathematical extensions to the multivariate QMOM method.

Task 2. Start to compile the necessary code to integrate the newly developed multivariate QMOM method into the SAP/SA software deliverable.

Year 3.
Task 1. Finish the theoretical development and software programming of the newly developed multivariate QMOM method.

Task 2. Compile technical reports and research papers on the newly developed multivariate QMOM method and their applications in aerosol simulation.

A Scalable and Extensible Earth System Model for Climate Change Science

A Proposal Submitted to the DOE Office of Science

Program Announcement:	LAB 06-04
Program Area:	Scientific Application: Climate Modeling and Simulation
Program Office:	Office of Biological and Environmental Research
Technical Contact:	Dr. Anjuli Bamzai

Applicant

Institution		*Principal Investigator*
OakRidge National Laboratory		John B. Drake
PO Box 2008, MS 6016		(865)574-8670
Oak Ridge, TN 37831-6016		drakejb@ornl.gov

Field Work Proposal ERKP576

Participating Institutions/Senior Personnel

***Lead PI:* John B. Drake, Oak Ridge National Laboratory**

***Co-Lead PI:* Phil Jones, Los Alamos National Laboratory**

Institution		*Senior Personnel*
Argonne National Laboratory (ANL)		Robert Jacob
Brookhaven National Laboratory (BNL)		Robert McGraw
Lawrence Berkeley National Laboratory (LBNL)		Inez Fung, Michael Wehner
Lawrence Livermore National Laboratory (LLNL)		Phillip Cameron-Smith, Arthur Mirin
Los Alamos National Laboratory (LANL)		Scott Elliot, Philip Jones, William Lipscomb, Mat Maltrud
National Center for Atmospheric Research (NCAR)		Peter Gent, William Collins, Tony Craig, Jean-Francois Lamarque, Mariana Vertenstein, Warren Washington
Oak Ridge National Laboratory (ORNL)		John B. Drake, David Erickson, W. M. Post, Patrick Worley
Pacific Northwest National Laboratory (PNNL)		Steven Ghan
Sandia National Laboratories (SNL)		Mark Taylor

Scientific Application Partnerships

Institution		*Principal Investigators*
Brookhaven National Laboratory		**Robert McGraw**
Lawrence Berkeley National Laboratory		Philip Colella
Lawrence Livermore National Laboratory		Dean Williams
Oak Ridge National Laboratory		Patrick Worley
University of Maryland		Eugenia Kalnay

Projected Funding Request: $6.6M per year for five years. This includes $4.3M U.S. Department of Energy Office of Biological and Environmental Research portion of collaborations with $2.3M in SciDAC SAP projects.