COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 02-2

NSF 01-171 **01/24/02**

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)

CHE - MAJOR RESEARCH INSTRUMENTATION (continued)

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(See GPG II.C For Definitions) ☐ FOR-PROFIT ORGANIZATION ☐ SMALL BUSINESS ☐ MINORITY BUSINESS ☐ WOMAN-OWNED BUSINESS

TITLE OF PROPOSED PROJECT **Acquisition of Computer Infrastructure for the SDSU Computational Science Research Center**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PREPROPOSAL NO., IF APPLICABLE
$ **225,643**	**36** months	**09/01/02**	

CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW

☐ BEGINNING INVESTIGATOR (GPG I.A)
☐ DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C)
☐ PROPRIETARY & PRIVILEGED INFORMATION (GPG I.B, II.C.6)
☐ HISTORIC PLACES (GPG II.C.9)
☐ SMALL GRANT FOR EXPLOR. RESEARCH (SGER) (GPG II.C.11)
☐ VERTEBRATE ANIMALS (GPG II.C.11) IACUC App. Date _____
☐ HUMAN SUBJECTS (GPG II.C.11)
Exemption Subsection _____ or IRB App. Date _____
☐ INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED (GPG II.C.9)
_____
☐ HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.E.1)

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COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) - continued from page 1
(Indicate the most specific unit known, i.e. program, division, etc.)

PHY - MAJOR RESEARCH INSTRUMENTATION
DBI - MAJOR RESEARCH INSTRUMENTATION

Project Summary

Funds are requested towards the purchase of a 100-processor Intel/Linux computer cluster and associated visualization workstations to support the combined research and educational mission of the SDSU Computational Science Research Center (CSRC). The CSRC is an interdisciplinary affiliation of faculty from the Departments of Astronomy, Biology, Chemistry, Computer Science, Geological Sciences, Mathematics, and Physics, and maintains distinct programs towards the M.S. and (beginning in Fall 2002) Ph.D. degrees. The majority of the research projects carried out under the auspices of the CSRC involve the application of numerical methods and/or extensive databases to problems in the natural sciences, including resource-intensive dynamics simulations and the analysis of high-volume visual data. The Linux cluster will become the primary computational resource of the CSRC, hosting research projects of the roughly forty participating faculty and their students in areas as diverse as quantum chemistry, cellular structure, hydrodynamics, and planetary astronomy. The proposed cluster will provide a central, high-performance facility dedicated to enhancing the research and instructional efforts of the CSRC member faculty. System and applications installation and maintenance will be carried out primarily by a full-time CSRC system administrator. Fourteen Intel graphics platforms will be housed in a computer classroom/visualization laboratory adjacent to the cluster, and made available to CSRC faculty and students for image manipulation in research and coursework. Six SGI Octane2's will also be purchased to serve those research groups with especially high graphics demands in each of the math and natural science departments currently bridged by the Center.

The projects carried out on these systems are expected to extend beyond those described here, and to evolve and diversify rapidly. For illustration, however, specific projects that could take immediate advantage of the equipment proposed for purchase include (i) calculation of structural and dynamical properties of reactive chemical intermediates with low-barrier mechanisms for chemical transformation; (ii) development of numerical integration techniques for application to oceanic flow patterns around static objects; (iii) modeling of protein-protein docking as a component in iterative protein design techniques; (iv) development and testing of mathematical models of flame dynamics; (v) simulation of collisions between different planets and between planets and their suns; (vi) calculation of dynamical properties in quantum fluids; (vii) three-dimensional mapping of mitochondrial structures and associated statistical analysis.

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B	Table of Contents (NSF Form 1359)	1	
C	Project Description (plus Results from Prior NSF Support) (not to exceed 15 pages) **(Exceed only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)**	15	
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*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

This proposal requests funds towards the purchase of a >100-processor Intel/Linux computer cluster and associated workstations for visualization, all in support of the research and training programs of the Computational Science Research Center (CSRC) at San Diego State University. The CSRC is an affiliation of roughly 40 faculty members from the Departments of Astronomy, Biology, Chemistry, Computer Science, Geological Sciences, Mathematics, and Physics under the direction of co-PI Castillo. The Center has offered an M.S. degree since Fall 2000 and has been approved to offer a Ph.D. degree program jointly with Claremont Graduate University beginning in Fall 2002. Sixteen students are already enrolled in the year-old M.S. program; a target of 70 graduate students is planned. The Center is described in greater detail on the web at http://www.sci.sdsu.edu/compsci/.

1 Results from Prior NSF Support

Cooksy was Co-PI on the NSF infrastructure instrumentation grant, "Acquisition of Computing Equipment for Computational Chemistry" (ARI-9512473; $115,552; S. R. Davis, PI), awarded to the University of Mississippi (UM). This grant funded the purchase of a four-processor SGI Power Challenge L computer and six peripheral SGI workstations, for the chemical modeling projects of the faculty and students of the UM Department of Chemistry. These computers were the principal tools in work presented in papers appearing in *J. Chem. Am. Soc.*, *J. Chem. Phys.*, *J. Phys. Chem.*, and other journals,[1–12] including work leading to four Ph.D. and two M.S. degrees (three by women, two by African Americans). This equipment continues to serve the UM chemistry research groups following Cooksy's departure for SDSU in 1999. Related educational activities include training graduate and undergraduate students in visualization and ab initio techniques in chemistry, and management of the Department's undergraduate computer lab. Summaries of the principal research projects supported follow.

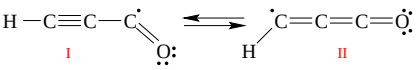
1.1 Hydrocarbon Strain Energies and Reactions with Oxygen (S. R. Davis)

The strain energies for several hydrocarbons up to six carbons were calculated using homodesmotic reactions and ab initio methods up to the CBS-Q level.[5] Of the non-composite methods, the MP2/6-311G(d,p) level gives the best overall agreement with QCISD(T)/6-311+G(2df,p) values, having a mean absolute deviation of only 0.36 kcal/mol, and agrees well with available experimental data. The strain energies for the two isomers of oxazetidine were also determined using isodesmic, homodesmotic, and hyperhomodesmotic models. Frequency analyses indicate that both isomers are stable.[4]

Equilibrium geometries for all reactants, products, and transition states in the three-step reaction of tetrafluoroethylene with O_2 were optimized and MP4//MP2 energies obtained. The $\cdot CF_2CF_2OO\cdot$ biradical was characterized for the first time and found to have C_s symmetry and a $^3A''$ ground electronic state, in contrast to the C_1 $\cdot CF_2OO\cdot$ biradical. The second step in the reaction was found to be rate-determining with an activation energy of 54.0 kcal/mol. The predicted reaction enthalpy of 62.7 kcal/mol agrees well with the experimental value of 66 kcal/mol. In a separate study, products of UV-photolyzed benzene/ozone and dimethylacetylene/ozone mixtures in 12 K argon matrices were characterized by comparison of observed IR spectra to ab initio frequencies and by CCSD(T)//MP2 transition state studies.[2,3] This allowed the unambiguous identification of the butadienylketene product and determination of a spin-crossing mechanism in the dimethylacetylene reaction to form dimethyloxirene.

1.2 Relocalization in Carbon-Chain Free Radicals (A. L. Cooksy)

Figure 1: Relocalization of HC_3O



Free radicals based on three- and four-atom carbon chains are central to the combustion mechanisms of numerous hydrocarbon fuels, and offer structural and dynamic challenges not seen in the well-studied smaller radicals. In addition to a tendency towards floppiness common in unsaturated carbon chains,[13] these radicals are subject to "relocalization" (Fig. 1). When a π bond adjoins a localized unpaired electron in one favorable canonical structure, there generally exists a second favorable structure that exchanges one end of the π bond for the unpaired electron.[14,15] This facile electron redistribution often separates configurational isomers of similar energy but differing substantially in bond order, geometry, and spin localization. Radicals with conjugated π-electron systems also tend to have low-lying electronic states, corresponding to excitations among the highest doubly-occupied, singly-occupied, and lowest unoccupied orbitals. Thermal vibrational or electronic excitations of many unsaturated intermediates in combustion and photolysis may therefore lead to significant shifts in electron density, and in turn to unexpected branching or redirection of product distributions.

Ab initio electronic structure calculations up to the CCSD(T) and multi-reference CI (MRCISD) levels have been carried out to ascertain the geometries, relative energies, isomerization barriers, and relevant spectroscopic properties of the lowest energy structural, configurational, and conformational isomers of C_3H_3O, C_4H_5, and a family of XCNY and XCCHY radicals.[9–12] Vibrational potential energy surfaces (PES) have been calculated along the two bending coordinates for H_2C_2HCO and H_2C_3HO and single coordinate of H_3C_3O that correlate with relocalization. Extremely large amplitude

bending motions are predicted for these three lowest energy structures, and at typical combustion temperatures it is likely that these molecules exist effectively as admixtures of two or more canonical forms. In contrast, 1,2-butadien-4-yl is the most stable of the butadienyl isomers by over 40 kJ/mol, indicating that cleavage of the weakest C-H bond in 1,3-butadiene results in a daughter radical with a bond order distribution and geometry substantially different from the parent. For nearly a third of the molecules studied, secondary relocalization isomers are found within 30 kJ/mol of the most stable state, suggesting that photolysis or pyrolysis of parent compounds may effectively result in multiple forms of the resulting reactive intermediates.

2 Research Activities

The equipment requested under the present proposal would be available to support all research programs affiliated with the CSRC. A few representative projects are described in detail below. Other projects are described at the CSRC website.

2.1 Computational Quantum Mechanics of Floppy Reactive Intermediates (A. L. Cooksy, Chemistry)

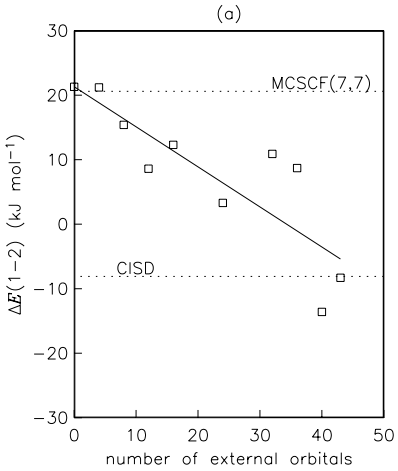
Cooksy's present work is an extension of the studies on floppy radical intermediates described in the preceding Section 1.2, and also includes several new projects in physical organic chemistry. Electronic structure studies continue for conjugated radicals of larger size and greater relevance to current synthetic and biochemical research. Simultaneously, the group is developing methods for studying the anharmonic vibrational dynamics of these systems along the coordinates of greatest interest.

The same features that lead to novel behavior of the floppy intermediates cause computational modeling of the electronic (and hence vibrational) wavefunctions to be problematic. A high degree of conjugation, and accompanying probability of spin contamination, suggest that approximations built on a single, unrestricted Hartree-Fock reference wavefunction will be inadequate, yet restricted Hartree-Fock wavefunctions offer a poor starting point for the description of conjugated electron systems. The C_4H_5 calculations described in the previous section found various levels of post-SCF theory could differ by as much as 70 kJ/mol on a given relative energy. Given that different configurations of the same structure are typically lie within 30 kJ/mol of each other, the accuracy of the computational methods is sorely tested by these systems.

2.1.1 Electronic Structure Calculations

Electronic wavefunctions and energies are calculated with widely-used quantum chemical packages.[16–18] A critical tool in identifying deficiencies of the available methods has been extension to MRCI, which allows contributions from both a large CASSCF active space of RHF configurations *and* single and double substitutions to high-lying virtual orbitals. Figure 2 illustrates the convergence of the multi-reference relative energy towards the CI results as substitutions to higher virtual orbitals are included.

Figure 2: Energy of $4a''$ C_2HO_2 relative to $5a''$ as a function of number of MRCISD external orbitals.



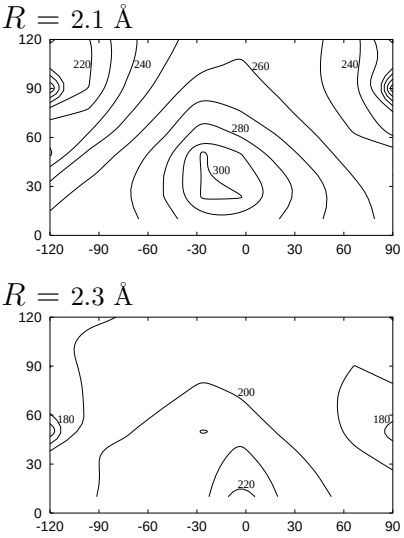
MRCI calculations will likely be essential for an adequate description of the larger conjugated radicals that comprise the next stage of investigation in these studies. As conjugation extends over greater distances, the excitation energy to the lowest lying spin states decreases, magnifying the impact of spin contamination in UHF-based wavefunctions, while the tendency of RHF wavefunctions to localize the electron distribution becomes correspondingly inappropriate. Spin contamination can be eliminated by using an ROHF reference wavefunction, but it then becomes especially important to employ a CI expansion that adequately represents the orbitals nominally associated with conjugation. The PI's group has found, for example, that the quartet spin state of the cyclononatetraenyl radical (C_9H_9) becomes more stable than the doublet at certain conformations. The relative energies of these states cannot be reliably estimated using the UHF-based coupled cluster methods that have proven so valuable up to this point. MRCISD calculations with a suitable (9,9) active space would resolve this, but exceed the resources available at SDSU.

Even for ground state properties, the volume of single-processor jobs appropriate to some projects is too daunting for the available systems. In the PI's recent study of the electrocyclic reactions of pentadienyl,[19] it was necessary to evaluate energies at over 100 points to sample a small three-dimensional section of the vibrational potential energy surface (Fig. 3) in order to ascertain the absence of a distinct disrotatory transition state. This was possible using semi-empirical AM1 calculations, but whether a corresponding map with reliable ab initio methods would have yielded the same results remains unproven.

2.1.2 Vibrational Dynamics Calculations

Single-point energy calculations along the floppy coordinate also allow qualitatively correct vibrational wavefunctions and energies to be calculated along the corresponding mode; the harmonic oscillator model assumed by electronic structure packages fails. This is particularly important when assessing computational results by comparison to the vibrationally-averaged constants available from spectroscopic data. The spectroscopic properties of these radicals will be highly sensitive to the curvature of the potential surface, and explicit dynamics calculations will yield the most reliable predictions to date for guiding experimental investigations into this fundamental class of reactive intermediate.

Figure 3: Sections of an AM1 surface for ring closure of pentadienyl to cyclopentenyl; axes are CH_2 dihedral angles relative to carbon chain.



The calculation of wavefunctions on anharmonic, multidimensional potential surfaces has been the subject of numerous studies, and several techniques are well-established,[20–23] although the application to large polyatomics remains somewhat problematic. However, the general formulation of the vibrational kinetic energy operator by Frederick and Woywood[24] allows the vibrational Hamiltonian to be written straightforwardly (if not easily) in terms of the internal coordinates that so clearly demark the relocalization pathway in these molecules. Because modes associated primarily with hydrogen atom motion remain significantly decoupled from the normal modes of the heavy-atom chain, this allows the Hamiltonian to be expressed in intuitive and fairly separable coordinates. The *ab initio* potential energy surface is likewise easily expressed in pointwise form along the internal coordinates, and accurate interpolation schemes exist if necessary.[25] Unlike many quantum dynamics studies, only the lowest energy states, up to the energies of any competing configurations or intervening barriers, remain of primary interest, and therefore extremely large vibrational basis sets are unnecessary. Treating only the internal coordinates of a four-atom chain, six coordinates are required, but in a local coordinate representation only four coordinates (two bond lengths and two bond angles) are strongly coupled to the relocalization pathways for the target species.[a] The qualitative accuracy desired may be achieved by a calculation significantly less demanding than the six-dimensional calculations carried out for water dimer,[26] or the exhaustive rovibrational analysis of the HOCl/HClO system.[27,28]

[a] For example, for H_2C_2HCO, the CCO angle and CC bond lengths vary by 130° and 0.1 to 0.2 Å, respectively, across the < 30 kJ/mol region of the surface. The other bond lengths in contrast vary by less than 0.025 Å, and the other bond angles by less than 12°.

Drawing on previous experience with the theory of effective Hamiltonians in floppy systems and the interpretation of spectroscopic data[7,29,30], the PI will calculate expanded four-dimensional potential energy surfaces for the two systems with the greatest body of existing experimental data: HC_3O and $H_2C_3HCH_2$. Ideally, these calculations take advantage of multiprocessor computers by running a large number of single-cpu jobs in parallel, rather than relying on per-job parallel execution. The collocation method[31] will initially be used to obtain vibrational wavefunctions on these surfaces. Collocation has the advantage over more sophisticated techniques of being mathematically transparent, easily programmed, and extremely efficient computationally. Although this has been applied primarily to weakly-bound complexes, in which the vibrational degrees of freedom lend themselves to an obvious separation scheme, it should be equally applicable to covalently bound polyatomics of similar dimensionality. If comparison to experimental rotational and hyperfine constants or vibrational transition energies indicates that higher accuracy is essential, the potential-optimized discrete variable representation[32–35] has provided a very successful approach to the *ab initio* determination of vibrational spectra in polyatomics. Furthermore, Poirier and Light have refined the methods whereby the multidimensional potential may be reduced to the necessary one-dimensional curves.[36] This combination of a general Hamiltonian and a pointwise integration algorithm should result in an efficient and widely applicable scheme for the evaluation of vibrational dynamics along the extremely anharmonic surfaces of these molecules.

This work has been supported by NSF, the Petroleum Research Fund, and the Exxon Education Foundation.

2.2 Microgravity Multiphase Dynamics (J. E. Castillo, Mathematics)

One area of Castillo's research is the development of high-order mimetic finite difference/volume methods. Mimetic difference approximations retain the symmetry properties of the continuum operators. Partial differential equations solved with mimetic difference approximations often automatically satisfy discrete versions of conservation laws and the continuumbased analogies to Stoke's theorem. Consequently, they are more likely to produce physically faithful results. These symmetries are easily preserved by local discrete high-order approximations on uniform grids, but are difficult to retain in high-order approximations on nonuniform grids. The main goal of this research is to construct local high-order mimetic difference approximations of differential operators on nonuniform grids. Local approximations only use function values at nearby points in the computational grid and are especially efficient on computers with distributed memory, such as the cluster proposed for purchase. High-order approximations can often be used to solve partial differential equation (PDEs) to a prescribed accuracy with only a

fraction of the grid points that would be required by a first- or second-order method.

A physical application of these methods is to fluid management in space-based systems of low gravity, especially combinations of a dispersed liquid or particulate solid in a continuous liquid or gas phase. The dispersed entities often interact with either with the walls of the container or with each other by virtue of their proximity. The handling and transfer of fluids from such systems requires an understanding of the behavior of the dispersed phase within the continuous phase. By quantifying the morphology of the combined system, we can design the techniques with which to contain, transport, and transfer those fluids. The objective of this research is to develop theoretical and computational models, assisted by ground-based experiments of the motion, deformation, and interaction of dispersed solid or liquid phases in the proximity of solid walls. The models will include surface tension effects to simulate the motion of immiscible fluids. The simulations will proceed in degree of complexity from dispersed spheres in two dimensional or axisymmetric flows to deforming dispersed fluid masses. In all cases, the interactions among dispersed elements and between them and the container walls will be considered. Code development has emphasized efficiency in parallel operation, and will benefit from the proposed cluster. This work is proposed for support from NASA; previous support for related projects has been from the US Army Research Office.

2.3 Novel Protein/Protein Docking by Design (J. J. Love, Chemistry)

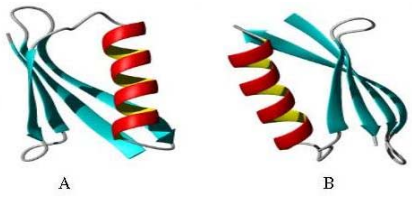
All organisms depend on the precise self-assembly of native proteins into functional multi-subunit complexes. The formation of these complexes is driven by the same forces that drive protein folding, in particular the hydrophobic effect,[37] as well as hydrophilic, electrostatic, hydrogen bonding, and dispersion forces. The goal of this work is to understand and control these forces, thereby designing proteins that self-assemble in predefined, structurally specific fashions. Understanding self-assembly and the noncovalent interactions that connect interacting molecular surfaces is a main focus of supramolecular chemistry.[38,39] Rather than using small organic molecules as building blocks, methods in this work mimic nature by employing protein-based building blocks, thereby exploiting the large body of physical data available for biological macromolecules. This method also enables the use of powerful *in vivo* genetic screens that can sample combinatorial libraries of up to 10^9 members for successful docking candidates.

The computational component of the docking strategy follows these steps: (*i*) Choose a small, monomeric protein and general target orientation for the docked complex; (*ii*) Computationally dock the backbones of the proteins in the target orientation and tabulate the atomic coordinates which result in maximal subunit-to-subunit surface complementarity; (*iii*) Treat the two molecules as one and use established protein design

algorithms[40] to repack the side-chains at the protein-protein interface in a manner similar to that observed in the cores of well-folded proteins.

A sample, successful application of this method work involves the 56-amino acid $\beta 1$ domain of the Streptococcal protein G, chosen because it has been extensively redesigned and biophysically analyzed,[41] expresses well in *e. coli*, is monomeric and well behaved in solution, and its compact structure has been determined to high resolution.[42,43] For the initial target orientation, a dual 180° rotation was carried out about the y and z axes, resulting in one molecule flipped head-to-tail and oriented helix-face to helix-face as shown in Fig. 4. Next, the interfacial space is searched for the optimal surface-to-surface geometric fit using the Geometric Recognition Algorithm (GRA), borrowed from the field of native protein docking.[44,45] The GRA treats the two molecules as rigid bodies and uses surface complementarity as the criteria for goodness of fit. The molecules are projected onto a three-dimensional grid of N^3 points and represented by the following discrete functions:

Figure 4: Initial target orientation of protein G dimer.



$$a_{l,m,n} = \begin{cases} 1 & \text{surface of molecule} \\ -15 & \text{inside the molecule} \\ 0 & \text{outside the molecule} \end{cases} \qquad b_{l,m,n} = \begin{cases} 1 & \text{surface/inside of molecule} \\ 0 & \text{outside the molecule} \end{cases}$$

Matching of complementary surfaces relies on optimization of the correlation function

$$c_{\alpha,\beta,\gamma} = \sum_{n=1}^{N} \sum_{m=1}^{N} \sum_{l=1}^{N} a_{l,m,n} \cdot b_{l+\alpha,m+\beta,n+\gamma}$$

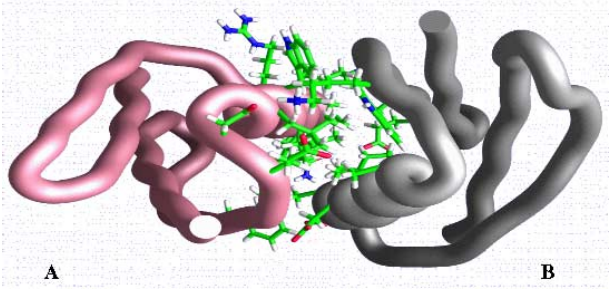
Even for a fixed relative orientation, high resolution calculation of the correlation function remains computationally intensive. The Fourier correlation theorem (FCT)[44] reduces roughly N^6 translational calculations down to the order of $N^3 \ln N^3$.[46,47] A single translational calculation with $N = 128$ took 25.4 days to complete on a single SGI R10000 processor without the FCT, and only 58 s with the FCT. On a Pentium IV, 1 GHz processor running Linux, the calculation now takes 11.5 s.

High resolution scans (i.e., 0.5 Å; 5°/scan) of 5,832 different rotational backbone positions take about 40 hours to complete. To prevent structural bias of the interface, the side-chain atoms of the wild-type residues were removed (except Cβ atoms). The coordinates of this optimized, docked complex were used in the next step of the computational docking process. The ORBIT suite of protein design algorithms[40] is used to perform side-chain selection on interfacial residue positions. The primary function of

these algorithms is to return a mutated protein sequence optimized for a given three-dimensional backbone structure (Street and Mayo, 1999). They employ an unbiased, quantitative design method based on the physical chemical properties that determine protein structure and stability.[48]

The RESLASS algorithm was used to determine which residues become buried ("core") upon docking, and which lie at the boundary. Fifteen residues in the present example were reclassified as core and seven as boundary. ORBIT was used to select hydrophobic side-chains for the interfacial core positions and hydrophilic side-chains for the reclassified boundary positions. Favorable interfacial proximity led two additional surface positions to be included. Figure 5 displays the side-chains of the 24 residues reclassified as a result of the dimerization. The total redesign resulted in a 20-fold mutant (12 for monomer A and 8 for B; 4 remained wild-type). Upon complex formation these mutant monomers bury about 1560 Å^2 of surface area (76% of which is hydrophobic). Experimental measurements of the mutated protein dimers will be used to assess the forces crucial to the self-assembly. This procedure is general, and the computational work, which is matched by experiments in Love's laboratory, can be expanded to numerous other protein systems with the proposed cluster computing and visualization resources. This work is supported by the Petroleum Research Fund.

Figure 5: Side chains affected by dimerization.



2.4 Nonlinear Dynamical Systems (A. Palacios, Mathematics)

The modeling of dense multiphase flow reactors is crucial for many energy conversion and chemical processing units. Typical examples of multiphase flow reactors include circulating fluidized-bed combustors and fluid catalytic cracking risers. The governing equations describing the phenomena inside multiphase flow reactors consist of a system of highly coupled partial differential equations. Solving these equations is a difficult and computionally intensive task. This research aims to develop a method to drastically reduce the computational effort required in modeling multiphase flow reactors. This reduction will be accomplished by developing a low order model based on the proper orthogonal decomposition (POD) method.

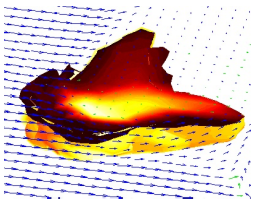
The POD is a procedure which provides a basis for the modal decomposition of spatio-temporal data obtained in the course of laboratory experiments or numerical simulations. The POD extracts key *spatial* ingredients from physical systems with spatial and tem-

poral characteristics. It produces basis functions which are then used to *dynamically* recreate the original data set. The essential advantage of the POD method is that it reduces a large set of partial differential equations to a smaller set of ordinary differential equations. This order reduction is valid because most of the energy of the eigenmodes is contained in the first few POD eigenmodes.

A reduced order model for multiphase flow reactors is being constructed using a state-of-the-art numerical algorithm developed by the National Energy Technology Laboratory for chemical reactions and heat transfer in dense or dilute fluid-solids flows. In addition, visualization tools are being developed for understanding the temporal behavior captured by the reduced order model. The specific objectives of this research project are: numerical generation of a database, which includes the spatial and temporal evolution of the relevant variables of the system; modal decomposition of relevant spatio-temporal variables; identification and separation of dominant spatial structures during the evolution of the fluid and solids phases; projections, via Galërkin methods, of the governing partial differential equations onto POD basis functions to produce the desired low-dimensional ordinary differential equations; and development of visualization tools for low order models. The development of the reduced order model and visualization tools will significantly impact the design of new reactors by improving the understanding of heat transfer and multiphase flow, making the parametric studies more affordable and helping to identify the dominant aspects of the critical mechanisms inside the reactor. This work is supported by the Department of Energy.

2.5 Simulations of Interplanetary and Solar/Planetary Collisions (E. Sandquist, Astronomy)

Figure 6: Distortion of Jupiter by collision with star.



The discovery of planets orbiting other stars in 1995 caused astronomers to re-examine their assumptions about how our own solar system formed. One area of research has involved the possibility that planets can strongly interact with their host stars. Many of the stars found to host newly discovered planets are found to have amounts of "heavy elements" (atomic numbers higher than helium) significantly higher than the average for stars near the Sun. In this research, hydrodynamical simulations probe whether giant planets similar to Jupiter or Saturn could be destroyed in the outer layers of a star, where the heavy elements they carry could pollute the gas in a way that could be observed by astronomers on Earth.[49] The simulations so far have focused on resolving the planet and examining its destruction in detail.[50] Because the planet's angular momentum is non-negligible relative to the star, more realistic simula-

tions would resolve both the planet and the star. This would increase the difficulty of the simulation because the problem is inherently three-dimensional and the size of the region that would have to be examined would need to be substantially larger than in current simulations. The proposed computing facility would make this kind of simulation practical. This work is supported by NSF.

A companion series of simulations examines the possible interaction between Earth-like planets and giant planets in young planetary systems. When a planetary system is still forming and finding a stable dynamical configuration, the orbits of small terrestrial planets can be perturbed to the point where they could collide with the host star or a giant planet. For a collision with a giant planet, the energy input could heat the planet and significantly increase its radius. Indeed, the first measurement of the radius of a giant planet around another star found an unusually large size for the planet's mass.[51]

2.6 Dynamics of Quantum Fluids (M. Boninsegni, Physics)

This research uses computer simulations to investigate the thermodynamic properties of fluids of interacting components, and correlates these with the fluid's quantum physics. Traditional approximate perturbative methods often prove inadequate here, due to the strong renormalization caused by interactions. The past two decades have witnessed the development of a powerful theoretical approach, fostered by the impressive progress of computer technology. The basic idea is that of formulating the many-body problem in a way suitable for a computer to solve exactly, i.e., with no approximation. A variety of computational methods have been developed in recent years, with notable success for a variety of such many-body problems. Examples of the systems studied are strongly correlated quantum fluids, such as liquid helium or the electron gas, quantum solids, such as helium and hydrogen at very high pressure, as well as quantum antiferromagnets, and in physical phenomena such as Bose-Einstein condensation, superfluidity and superconductivity. These simulations presently occupy the group's 20-cpu linux cluster, and the increased resources proposed for purchase would allow the systems under study to expand. This work is supported by NSF and the Petroleum Research Fund.

2.7 Mitochondrial Structure and Function (T. Frey, Biology)

The emphasis of this research program is on the function of mitochondria revealed in their structure and dynamics.[52–55] Mitochondria are subcellular organelles that provide chemical energy in the form of ATP (adenosine triphosphate) to cells by oxidizing carbohydrates and fatty acids in a mechanism analogous to a hydrogen/oxygen fuel cell. State-of-the-art microscopy provides the principal research tool for determining the mitochon-

drial structure. Conventional, thin-section electron micrographs are analyzed in conjunction with three-dimensional electron tomograms, derived from a series of thick-section (0.25-0.50 μ) electron micrographs recorded from a single specimen as it is tilted in 1-2 degree increments (Fig. 7). Calculation of the tomogram image from the micrographs can be a very time consuming step for large images (a typical tomogram will contain 256^3 to 512^3 voxels, and some as many as 1024^3), especially when more complicated image-interpolation algorithms are used. Fortunately, the process is inherently parallelizable as a series of two-dimensional reconstructions from one-dimensional projections. Even then, manipulation of these volumes in real time has been limited by the available hardware. Interpretation of the final tomogram is, at present, time consuming as it requires hand tracing of structural features such as the membrane profiles in each of hundreds of layers within each tomogram. An automated tracing algorithm is being developed that will demand high-performance computation, owing to the sophistication of the algorithm and the large amount of data. The automated tracing algorithm will also be applied hundreds of images of mitochondria observed in thin sections of cells in order to create a statistically significant sample of structural features. These features are used in turn as diagnostics for physiopathology of the mitochondria, including loss of membrane potential, swelling, release of cytochrome c to initiate apoptosis, and cessation of protein importation. This work is supported by the American Heart Association.

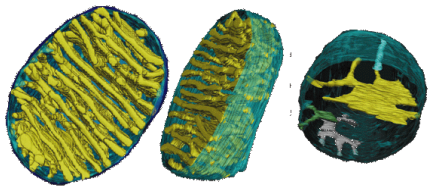


Figure 7: Digitized 3-D mapping of mitochondrial tomogram.

3 Description of the Research Instrumentation and Needs

The equipment proposed for purchase is a Western Scientific KiloCluster model computer cluster of over 100 Intel Pentium processors, including a dual processor master node. Currently, the Pentium III 1.13 GHz Tualatin processors offer the optimal combination of cost, subsystem compatibility, and speed. The quoted system will have a floating point processing speed of roughly 300 Gflop/s. Processors are housed in shared-memory pairs on Tyan 2518 motherboards, which offer a 133 MHz bus speed and memory expansion up to 4 GB. The expected demands of the programs allow each node to be limited initially to 1 GB of memory and a 20 GB IDE hard drive. Because the overall data storage requirements for current projects are not enormous, hard disk volume will to some extent be sacrificed to improve the access speed for those projects that rely heavily on disk storage of scratch data. User applications and data files will

reside primarily on one of two 100 GB hard disks connected to the master node. Daily incremental and weekly full backups of user files to a remote site will be accomplished through a standard implementation of the NFS package available with Linux. Western Scientific is the selected vendor because of its reputation and visibility in large-cluster assembly, and its location in San Diego simplifies installation and initial maintenance. The operating system will be RedHat Linux, with which the majority of CSRC users are already familiar, and which any competitive developer of research-grade software is supporting. The bulk of the software development will take advantage of the free GNU C and Fortran compilers. Individual research groups and departments will be expected to provide funds as necessary to secure licenses for any commercial compilers or math subroutine libraries, although additional funds may be provided from the CSRC budget at the Director's discretion. A Cyclades TS-series terminal server will enable robust management of the nodes, facilitating rapid turn-around in the event of node failure.

The graphics workstations proposed for visualization are divided into two groups: six entry-level SGI Octane-2 systems for use in research projects with an integral dependence on high-resolution image manipulation, and 14 Intel-based Western Scientific Xfusion systems for more routine graphics capability, including coursework. The SGI's will be purchased with single R12000A 360MHz MIPS processors, 256 MB RAM, 18 GB hard disk, and 21-inch monitors. These workstations remain arguably the most advanced desktop visualization tools available. In addition, the quality engineering of all components in the system architecture (64-bit processors, 1.6 GB/s I/O bandwidth) make these extremely powerful and flexible machines for single-processor, computationally demanding jobs. The Intel machines are based on single, 2.0 GHz Pentium IV processors, 1.0 GB RAM, and GeForce 3-D video cards.

Central computing facilities provided by the CSRC presently consist of a four-processor Compaq Alpha/Linux system and 12 Intel/Windows desktop computers, all centrally located in the Physics building. While the Alpha cluster is extremely fast for floating-point operations, the number of processors is insufficient to support the volume of jobs faculty would like to run, and software development for the Alpha chip has always lagged the Intels. The Windows machines are primarily for student use in running applied math software (e.g., MatLab and Maple) for analysis of research results or carrying out projects related to coursework. The facilities are not intended to serve classroom functions, as will the proosed Xfusion systems. SDSU faculty are also eligible to apply for time at the San Diego Supercomputing Center, which hosts the 1152-cpu BlueHorizon IBM SP cluster. While this system remains available for the most demanding jobs, it is not specifically intended to further the educational missions of participating institutions, and support of software applications and user accounts is relatively limited. For exam-

ple, new accounts are approved only twice a year, and applications that have not been optimized for parallel execution (such as Gaussian 98) are unsupported. Data storage is limited to 100 MB per account and backup is solely the user's responsibility. In addition, the resource is heavily used, and jobs requesting more than 2 hours of real time are typically in queue for one to two days; this can seriously impede code development.

4 Impact of Infrastructure Projects

The CSRC's principal goal is the advancement of computational science as an interdisciplinary venture. It accomplishes this by sponsoring degree programs, courses, seminars, and research activities, all founded on interaction among SDSU's natural scientists and applied mathematicians. Yet it does not now offer a shared computational research facility equal to the demands of the participating faculty and students. Funding this proposal will establish such a facility, which will identify common threads in methodology, reduce redundant efforts to procure computer time at off-campus facilities, provide a training resource for students, and further the research efforts. A system administrator and three graduate student trainees will manage user requests for software support and development, and bring opportunities for collaboration to the attention of the researchers.

As a recruitment and training tool, the cluster and visualization equipment will play a major role in the development of the CSRC. It is now the norm for prospective students and faculty in the natural sciences to employ computational methods as a substantial component of their research, and any canny visitor investigating the viability of SDSU as a home for their research training or advancement will inquire as to the availability of on-site, research-grade computational equipment. It falls naturally to CSRC to ensure that our University can satisfy any such inquiry by providing equipment of the level requested in this proposal.

In addition, the impact of a strengthened infrastructure in the CSRC benefits minority students by virtue of SDSU's leadership in minority recruiting in California. The CSRC serves undergraduate and graduate students of SDSU by offering an emphasis in computational science for B.S. Applied Mathematics candidates, and M.S. and (as of Fall 2002) Ph.D. degree programs. Aggressive outreach efforts have resulted in over 45% of the overall student population representing underserved minorities. Freshman admissions to the University in Fall 2000 included over 2500 Latinos and Mexican Americans, nearly 700 African Americans, and nearly 100 Native Americans. Just over half of the student population are women. The College of Sciences manages fourteen distinct programs to promote the participation of underrepresented groups in the sciences, including the Minority Access to Research Careers (MARC) program which places minority un-

dergraduate students in research traineeships with the specific goal of developing their skills, confidence, and interest for pursuing advanced degrees in the natural sciences. The PI and other members of the CSRC have sponsored students in the MARC program.

5 Project and Management Plans

The cluster and visualization lab machines will reside in room 121 (960 sq.ft.) of the Physics/Astronomy Building, centrally located to the CSRC participating departments. The roughly 50 kBTU in heat generated by all these systems can be accommodated by the existing air conditioning system, but room renovations to improve the hardware capacity are planned before installation in any case. Batch job scheduling and launching on the cluster will be handled using the free MauiScheduler software, which guards against excessive use by a single account to the exclusion of others. A full-time CSRC system administrator, to be hired in summer 2002, will handle all routine support and maintenance of these systems. The Xfusion workstations will be available at all times by card-key access to the CSRC students and faculty; the cluster will be partitioned off and available for physical access only by the sysadmin and assistants. The six SGI Octane-2 workstations will be made available to researchers in the each of the six mathematics and natural sciences departments. Each of the Octanes must be generally accessible to all CSRC researchers in that department, but will be under the supervision of those faculty who rely regularly on high performance graphics tools in their research (e.g., Cooksy and Love in Chemistry, Palacios in Mathematics, Sandquist in Astronomy, Frey in Biology). CSRC faculty routinely manage their own Unix systems already. When needed, assistance can be obtained from the CSRC sysadmin, graduate assistants, or the College of Sciences computer support group. SDSU's full-time computer security technician will be called on for assistance in that arena.

The CSRC sysadmin will handle routine issues of resource allocation involving the cluster and Xfusion machines. For example, some part of the cluster's resources may be reserved in order to meet a deadline, and the Xfusions will be dedicated to scheduled coursework at prearranged times. The CSRC sysadmin will be expected to approve any such course-related request, and research-related requests that will not delay batch submissions on the cluster by more than a day. The sysadmin will consult Cooksy if such requests are too frequent or would significantly delay current batch requests. Cooksy, in consultation with the co-PI's, will decide any questions arising from the distribution of equipment. Love will serve in the same capacity with regard to software purchases from CSRC funds. As Director of the Center, Castillo will supervise the project personnel and has ultimate authority over CSRC resource allocations.

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(1) "Relocalization in floppy free radicals: the OCNO and OCCHO isoelectronic series," A.L. Cooksy, *J. Am. Chem. Soc.* **123**, 4003–4013 (2001).

(2) "Ab initio study of the C_4H_5 isomers," C.L. Parker and A.L. Cooksy, *J. Phys. Chem. A* **103**, 2160–2169 (1999).

(3) "Relocalization in Floppy Free Radicals: *Ab Initio* Calculations of the C_3H_3O Isomers," A.L. Cooksy, *J. Phys. Chem.* **102**, 5092–5099 (1998).

(4) "Calculations on Ground and Excited State Potential Energy Surfaces of Floppy Free Radicals: HC_4H_2, HC_3NH, and HC_3O," H. Wang and A.L. Cooksy, *Chem. Phys.* **213**, 139–151 (1996).

(5) "Conjugated π-Electron Systems in Reactive Molecules: Multiple Minima on $^2A'$ Potential Surfaces of Carbon Chain Free Radicals," A.L. Cooksy, *J. Am. Chem. Soc.* **117**, 1098–1104 (1995).

Additional:

(1) "Structures and Properties of the 1,3-Butadienyl Radicals," C.L. Parker and A.L. Cooksy, *J. Phys. Chem.* **102**, 6186–6190 (1998).

(2) "Structures, Electronic Properties, and Isomerization of the HCCCO Radical," A.L. Cooksy, F.-M. Tao, W. Klemperer, and P. Thaddeus, *J. Phys. Chem.* **99**, 11095–11100 (1995).

(3) "The fine structure intervals of N^+ by far infrared laser magnetic resonance," J.M. Brown, T.D. Varberg, K.M. Evenson, and A.L. Cooksy, *Astrophys. J.* **428**, L37–L40 (1994).

(4) "The structure of the HCCCO radical: rotational spectra and hyperfine structure of monosubstituted isotopomers," A.L. Cooksy, J.K.G. Watson, C.A. Gottlieb, and P. Thaddeus, *J. Chem. Phys.* **101**, 178–186 (1994).

(5) "Dipole Moment Analysis of Excited van der Waals Vibrational States of ArHCl," A.L. Cooksy, M.J. Elrod, R.J. Saykally, and W. Klemperer, *J. Chem. Phys.* **99**, 3200–3204 (1993).

d. **Synergistic Activities:**

(1) Development of an innovative, intuition-based physical chemistry course for undergraduates, with accompanying textbook.

(2) Numerous studies integrating the fields of laboratory spectroscopy and molecular astrophysics, including: first direct measurement of fine structure intervals in atomic ions, used in the astrophysical analysis of massive objects near the galactic center and in the study of cool atomic interstellar gas clouds; development of the Berkeley infrared spectrometer for studies of refractory element clusters in supersonic jets, used to obtain the first infrared spectra of pure carbon compounds found in carbon star circumstellar envelopes; pure rotational spectroscopy and structure determination of candidates for observation in cold pre-stellar clouds.

(3) Co-authorship of collaborative proposals to support departmental and university-wide academic infrastructure at U. Mississippi.

e. **Collaborators and Affiliations:**

Collaborators last 48 months

W. Chen (Wesleyan College Chemistry)
S. R. Davis (U. Miss. Chemistry)
C. A. Gottlieb (Center for Astrophysics)
D. B. Grotjahn (SDSU Chemistry)
M. C. McCarthy (Center for Astrophysics)
S. E. Novick (Wesleyan College Chemistry)
M. J. Travers (Center for Astrophysics)
J. Vrtílek (Goddard Center, NASA)
L. M. Ziurys (U. Arizona Chemistry/Astronomy)
John Love (SDSU)
Jose Castillo (SDSU)

Students advised last 5 years

A. J. Grayson (US Patent Office)
C. L. Parker (National Cancer Institute)
H.-B. Wang (U. Miss. Information Technology)
C. Martinez (SDSU Chemistry)
C. Hinton (SDSU Chemistry)
R. Wong (SDSU Chemistry)
D. Xu (SDSU CSRC)

Totals: 7 graduate students; 0 postdocs.

Advisors

- R. J. Saykally (U. C. Berkeley Department of Chemistry)
- P. Thaddeus (Harvard-Smithsonian Center for Astrophysics)
- W. Klemperer (Harvard University Department of Chemistry)

Jose E. Castillo

Department of Mathematics
San Diego State University
San Diego CA 92182-7720

phone: 619-594-7205
fax: 619-594-6746
e-mail: castillo@myth.sdsu.edu

a. **Professional Preparation:**

Universidad Central de Venezuela	mathematics	B.S. 1978
University of Texas, Austin	mathematics	M.S. 1984
University of New Mexico	mathematics	Ph.D. 1987

b. **Appointments:**

- **1992**– : Associate Professor, Department of Mathematics, San Diego State University.
- **1987–1992**: Assistant Professor, Department of Mathematics, San Diego State University.

c. **Publications:** Related:

(1) "Numerical simulation of the flow past a sphere in vertical motion within an stratified fluid," C.R. Torres, J. Ochoa, J.E. Castillo, and H. Hanazaki, *J. Comp. Appl. Math.* **103**, 1 (1999).

(2) "A Generalized Length Strategy for Direct Optimization in Planar Grid Generation," J.E. Castillo and J.S. Otto, *Math. and Comp in Simulation* **44**, 441-456 (1997).

(3) "Solution Adaptive Discrete Variational Grid Generation for Fluid Flow Calculations," J.E. Castillo and E. Pedersen, *J. Comp. Appl. Math.* **97**, 343-370 (1996).

(4) "The Sensitivity and Accuracy of Fourth Order Finite-Difference Schemes on Nonuniform Grids in One Dimension," J.E. Castillo, M. Shashkov, J.M. Hyman, and S. Steinberg, *Comp. Math. Appl.* **30**, 41-55 (1995).

(5) "An Adaptive Direct Variational Grid Generation Method," J.E. Castillo, *Comp. Math. Appl.* **4**, 1 (1991).

Additional:

(1) "A Practical Guide to Planar Grid Generation," J.E. Castillo and J.S. Otto, *Comp. Math. Applic.* **37**, 123–156 (1999).

d. **Synergistic Activities:**

(1) Founder and Director of the Computational Science Research Center at San Diego State University.

(2) PI for the NSF-funded Pan-American Workshops on Computational and Applied Mathematics, 1992 and 1998.

(3) Collaborative research projects with Los Alamos National Laboratory on the development of adaptive grid generation and high-order finite difference schemes.

e. **Collaborators and Affiliations:**

Collaborators last 48 months

J.S. Otto (LANL)
J. Ochoa (CICESE, Tijuana-Ensenada Mexico)
Hideshi Hanazaki (Natl Inst Env Stud, Ibaraki, Japan)
John Love (SDSU)
Andrew Cooksy (SDSU)

Students advised last 5 years

Carlos Torres (Ensenada, Mexico)
Jonathan Richardson (SDSU)
Sharon Won (SDSU)
T. McGuinness (SDSU)

Totals: 10 graduate students; 0 postdocs.

Advisors

- Stanly Steinberg (University of Texas, Austin)
- Patrick Roache (University of New Mexico)

John J. Love

Department of Chemistry
San Diego State University
San Diego CA 92182-1030

phone: 619-594-2063
fax: 619-594-4634
e-mail: jlove@sciences.sdsu.edu

a. **Professional Preparation:**

SUNY Stony Brook	biochemistry	B.S. 1991
University of California, San Diego	biochemistry	Ph.D. 1999
Scripps Research Institute, San Diego	DNA structure	1998–1999
California Institute of Technology	protein engineering	1999–2001

b. **Appointments:**

- **2001**–: Assistant Professor, Department of Chemistry, San Diego State University.

c. **Publications:** Additional:

(1) "Structural Basis for DNA Bending by the Architectural Transcription Factor LEF-1," J. Love, X. Li, D. A. Case, K. Giese, R. Grosschedl, and P. E. Wright, *Nature* **376**, 791 (1995).

(2) "Multimedia Chemistry Lectures," R. M. Whitnell, E. A. Fernandes, F. Almassizadeh, J. J. Love, B. M. Dugan, B. A. Sawrey, and K. R. J. Wilson, *J. Chem. Ed.* **71**, 721 (1994).

d. **Collaborators and Affiliations:**

Collaborators last 48 months	**Students advised last 5 years**
Alex Burgin (Emerald Biosciences)	Jennifer Reichert (SDSU)
Peter Dervan (CalTech)	Mina Stemm (SDSU)
Adam Urbach (CalTech)	Mark Griffith (SDSU)
Peter Wright (Scripps)	Ushma Shukla (SDSU)
H. Jane Dyson (Scripps)	Nora Barakat (SDSU)
John Chung (Scripps)	Charlene Hooper (SDSU)
Xiang Li (Boeringer Ingleham)	Tarah Rempel (SDSU)
Joel Gottesfeld (Scripps)	
David Millar (Scripps)	
Andrew Cooksy (SDSU)	
Jose Castillo (SDSU)	

Totals: 5 graduate students; 0 postdocs.

Advisors

- S. L. Mayo (California institute of Technology)
- P. E. Wright (Scripps Research Institute)
- E. Komives (U. C. San Diego)

Antonio Palacios

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San Diego State University
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a. **Professional Preparation:**

LaSalle University	computer science	B.S. 1986
Arizona State University	computational mathematics	M.S. 1990
Arizona State University	computer science	M.S. 1994
Arizona State University	applied mathematics	Ph.D. 1995
University of Houston	physics and mathematics	1996–1999

b. **Appointments:**

- **1999**– : Assistant Professor, Department of Mathematics, San Diego State University.
- **1995–1996**: Research Scientist, Computer Graphics Laboratory, Hewlett-Packard Co.

c. **Publications:** Related:

(1) "Heteroclinic cycles in rings of coupled cells," P.-L. Buono, M. Golubitsky, and A. Palacios, *Physica D.* **143**, 74–108 (2000).

(2) "Integrating the Kuramoto-Sivashinsky equation in a circular domain," D. Zhang, G. Wei, D. Kouri, D. Hoffmann, A. Palacios, M. Gorman, and G. Gunaratne, *Phys. Rev. E* **60**, 3353–3360 (1999).

(3) "Modal decomposition of hopping motion in cellular flame patterns," A. Palacios, G. Gunaratne, and M. Gorman, *Chaos* **9**, 755–767 (1999).

(4) "A Karhunen-Loève analysis of spatiotemporal flame patterns," A. Palacios, G. Gunaratne, M. Gorman, and K. Robbins., *Phys. Rev. E* **57**, 5958–5971 (1998).

(5) "Cellular pattern formation in circular domains," A. Palacios, G. Gunaratne, M. Gorman, and K. Robbins, *Chaos* **7**, 463–475 (1997).

Eric L. Sandquist

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San Diego State University
San Diego CA 92182-1221

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a. **Professional Preparation:**

University of Virginia	physics	B.A. 1991
U. C. Santa Cruz	astronomy	M.S. 1993
U. C. Santa Cruz	astronomy	Ph.D. 1996

b. **Appointments:**

- **1999**– : Assistant Professor, Department of Astronomy, San Diego State University.
- **1999–1999**: Lecturer, Department of Astronomy, Northwestern University.

c. **Publications:** Related:

(1) "On the Formation of Helium Double Degenerate Stars and Pre-Cataclysmic Variables," E.L. Sandquist, R.E. Taam, and A. Burkert, *Astrophys. J.* **533**, 984–997 (2000).

(2) " Double Core Evolution X. Through the Envelope Ejection Phase," E.L. Sandquist, R.E. Taam, X. Chen, P. Bodenheimer, and A. Burkert, *Astrophys. J.* **500**, 909–922 (1998).

(3) "Planet Consumption and Stellar Metallicity Enhancements," E.L. Sandquist, R.E. Taam, D.N.C. Lin, and A. Burkert, *Astrophys. J.* **506**, L65–L68 (1998).

(4) "Composition Mixing during Blue Straggler Formation and Evolution," E.L. Sandquist, M. Bolte, and L. Hernquist, *Astrophys. J.* **477**, 335–345 (1997).

(5) "CCD Photometry of the Globular Cluster M5. I. The Color-Magnitude Diagram and Luminosity Functions," E.L. Sandquist, M. Bolte, P. Stetson, and J. Hesser, *Astrophys. J.* **470**, 910–952 (1996).

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San Diego State University
San Diego CA 92182-1233

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a. **Professional Preparation:**

Universita' degli studi di Genova	physics	B.S. 1986
Florida State University	physics	Ph.D. 1992
NCSA	condensed matter physics	1992–1995
University of Delaware	condensed matter physics	1995–1997

b. **Appointments:**

- **2001**– : Associate Professor, Department of Physics, San Diego State University.
- **1997–2001**: Assistant Professor, Department of Physics, San Diego State University.

c. **Publications:** Related:

(1) "Phase Separation in Mixtures of Hard Core Bosons," M. Boninsegni, *Phys. Rev. Lett.* **87**, 201 (2001).

(2) "Ab Initio Potentials and the Equation of state of Condensed Helium at High Pressure," S. Y. Chang and M. Boninsegni, *J. Chem. Phys.* **115**, 2629 (2001).

(3) "Helium in one-dimensional nanopores: Free dispersion, localization and commensurate/incommensurate transition with nonrigid orbitals," M. Boninsegni, S.-Y. Lee and V. H. Crespi, *Phys. Rev. Lett.* **86**, 3360 (2001).

(4) "Condensation of Helium in Nanotube Bundles," M. W. Cole, V. H. Crespi, G. Stan, C. Ebner, J. Hartman, S. Moroni and M. Boninsegni, *Phys. Rev. Lett.* **84**, 3883 (2000).

(5) "Equation of State of Solid ^{3}He," S. Moroni, F. Pederiva, S. Fantoni and M. Boninsegni, *Phys. Rev. Lett.* **84**, 2650 (2000).

Terrence G. Frey

Department of Biology
San Diego State University
San Diego CA 92182

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fax: 619-594-5676
e-mail: tfrey@sunstroke.sdsu.edu

a. **Professional Preparation:**

Ohio State University	chemistry	B.S. 1970
UCLA	biochemistry	Ph.D. 1975
Universitat Basel, Switzerland	physical biochemistry	1975–1977
Duke University Medical Center	physical biochemistry	1977–1978

b. **Appointments:**

- **1995**– : Associate Chair, Department of Biology, San Diego State University.
- **1988**– : Professor, Department of Biology, San Diego State University.
- **1986–1988**: Associate Professor, Department of Biology, San Diego State University.
- **1984–1986**: Research Associate Professor, Department of Biochemistry and Biophysics, University of Pennsylvania
- **1978–1984**: Research Assistant Professor, Department of Biochemistry and Biophysics, University of Pennsylvania

c. **Publications:** Related:

(1) "Electron Tomography of Neuronal Mitochondria:Three-dimensional structure and organization of cristae and membrane contacts," G. Perkins, C. Renken, M. E. Martone, S. J. Young, M. Ellisman, and T. G. Frey, *J. Struct. Biol.* **119**, 260–272 (1997).

(2) "Electron Tomography of Mitochondria from Brown Adipocytes Reveals Crista Junctions," G. Perkins, J. Song, L. Tarsa, T. Deerinck, M. Ellisman, and T. G. Frey, *J. Bioenergetics and Biomembranes* **30**, 431–442 (1998).

(3) "The Internal Structure of Mitochondria," T. G. Frey and C. A. Mannella, *Trends Biochem. Sci.* **25**, 319–324 (2000).

(4) "Recent Structural Insight into Mitochondria Gained by Microscopy," G. A. Perkins and T. G. Frey, *Micron* **31**, 97–111 (2000).

(5) "Electron Tomography of Mitochondria After the Arrest of Protein Import Associate d with Tom 19 Depletion," G. A. Perkins, C. W. Renken, I. J. van der Klei, M. H. Ellisman, W. Neupert, and T. G. Frey, *Eur. J. Cell Biol.* **80**, 139–150 (2001).

CSRC System Administrator

This individual will be primarily responsible for the requested equipment. This position has been announced open for hiring, to be filled by July 1, 2002.

The following characteristics are specified in the position announcement.

a. **Professional Preparation:**

- Equivalent of M.S. or Ph.D. in computational sciences plus five years experience in the area.
- Two years experience in programming, system administration, and/or hardware support, including one year of operating system design, modification, installation, and/or evaluation.

b. **Specialized Skills:**

- Programming or scripting in: Fortran90, C, C++, Java, Expect, Bash, Perl.
- Fluent with Unix, Windows, MacOS.
- Extensive experience with Linux kernel and Linux networking management, including cluster management.
- Familiarity with high-performance computing compilers, libraries, parallel processing management, and debugging software.
- Demonstrated success in technical education and training.

SUMMARY PROPOSAL BUDGET

YEAR 1

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **San Diego State University Foundation**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Andrew L Cooksy**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Andrew L Cooksy - Principal Investigator**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Jose E Castillo - Co-PI**	**0.00**	**0.00**	**0.00**	**0**	
3. **John Love - Co-PI**	**0.00**	**0.00**	**0.00**	**0**	
4.					
5.					
6. (**0**) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**3**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.)					
108-proc Kilocluster $ **117,378**					
14 Xfusion workstations **18,875**					
6 SGI Octane-2's **89,390**					
TOTAL EQUIPMENT				**225,643**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**0**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**0**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**225,643**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) **MTDC (Rate: 51.0000, Base: 0)**					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**225,643**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **225,643**	$

M. COST SHARING PROPOSED LEVEL $ **100,000** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY
Andrew L Cooksy		INDIRECT COST RATE VERIFICATION
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked / Date Of Rate Sheet / Initials - ORG
Feinberg, Lawrence		

SUMMARY PROPOSAL BUDGET

Cumulative

FOR NSF USE ONLY		
PROPOSAL NO.	DURATION (months) Proposed	Granted
AWARD NO.		

ORGANIZATION: **San Diego State University Foundation**

PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR: **Andrew L Cooksy**

A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)	NSF Funded Person-mos. CAL	ACAD	SUMR	Funds Requested By proposer	Funds granted by NSF (if different)
1. **Andrew L Cooksy - Principal Investigator**	**0.00**	**0.00**	**0.00**	$ **0**	$
2. **Jose E Castillo - Co-PI**	**0.00**	**0.00**	**0.00**	**0**	
3. **John Love - Co-PI**	**0.00**	**0.00**	**0.00**	**0**	
4.					
5.					
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)	**0.00**	**0.00**	**0.00**	**0**	
7. (**3**) TOTAL SENIOR PERSONNEL (1 - 6)	**0.00**	**0.00**	**0.00**	**0**	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (**0**) POST DOCTORAL ASSOCIATES	**0.00**	**0.00**	**0.00**	**0**	
2. (**0**) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	**0.00**	**0.00**	**0.00**	**0**	
3. (**0**) GRADUATE STUDENTS				**0**	
4. (**0**) UNDERGRADUATE STUDENTS				**0**	
5. (**0**) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)				**0**	
6. (**0**) OTHER				**0**	
TOTAL SALARIES AND WAGES (A + B)				**0**	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				**0**	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)				**0**	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5,000.) **$ 225,643**					
TOTAL EQUIPMENT				**225,643**	
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)				**0**	
2. FOREIGN				**0**	
F. PARTICIPANT SUPPORT COSTS					
1. STIPENDS $ **0**					
2. TRAVEL **0**					
3. SUBSISTENCE **0**					
4. OTHER **0**					
TOTAL NUMBER OF PARTICIPANTS (**0**) TOTAL PARTICIPANT COSTS				**0**	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				**0**	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				**0**	
3. CONSULTANT SERVICES				**0**	
4. COMPUTER SERVICES				**0**	
5. SUBAWARDS				**0**	
6. OTHER				**0**	
TOTAL OTHER DIRECT COSTS				**0**	
H. TOTAL DIRECT COSTS (A THROUGH G)				**225,643**	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)					
TOTAL INDIRECT COSTS (F&A)				**0**	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				**225,643**	
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)				**0**	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)				$ **225,643**	$

M. COST SHARING PROPOSED LEVEL $ **100,000** AGREED LEVEL IF DIFFERENT $

PI / PD TYPED NAME & SIGNATURE*	DATE	FOR NSF USE ONLY
Andrew L Cooksy		INDIRECT COST RATE VERIFICATION
ORG. REP. TYPED NAME & SIGNATURE*	DATE	Date Checked / Date Of Rate Sheet / Initials - ORG
Feinberg, Lawrence		

NSF Form 1030 (10/99) Supersedes all previous editions

C***SIGNATURES REQUIRED ONLY FOR REVISED BUDGET (GPG III.B)**

Budget Justification

- **B. Other Personnel: CSRC System Administrator.** This is a full-time position that has been approved for hire in the fiscal year beginning July 1, 2002 at an annual salary of $70,000 with additional 33% funding for fringe benefits, totaling $93,333/year. This staff position is a specific component of the annual budget approved by the SDSU Division of Academic Affairs to the CSRC, and co-PI Castillo as CSRC Director manages those funds and will oversee the hiring. Although this Administrator will have functions outside the scope of this proposal, the systems proposed for purchase will constitute the principal computer resources of the CSRC, and are expected to demand the majority of the Administrator's time. One quarter of the funding for this position over the three year period of the grant – a total of $70,000 – is offered as part of the matching commitment from SDSU towards this proposal, as indication of the University's intention and ability to supply adequate staffing towards the support of the instrumentation. No funds are requested from NSF for this position.

- **D. Equipment.**

  1. **Western Scientific Intel Kilocluster.** This is the proposed Intel/Linux cluster that will be the centerpiece computing facility for CSRC research. Requested funds are based on the vendor's quote provided in the Supplementary Documentation section of this proposal, with 7.75% sales tax added. As a local firm, Western Scientific will waive delivery charges for this equipment. This will be purchased with the requested NSF funds.

  2. **6 SGI Octane-2's.** These are the research-grade graphics workstations that are intended to address the needs among CSRC researches for routine access to high performance visualization tools. Requested funds are based on the vendor's quote provided in the Supplementary Documentation section of this proposal, with added 7.75% sales tax and shipping charges of $120/ea. (based on vendor's estimate). These will be purchased with the requested NSF funds.

  3. **14 Western Scientific Xfusion workstations.** These are the Intel graphics workstations that will comprise the proposed visualization classroom and laboratory. Requested funds are based on the vendor's quote provided in the Supplementary Documentation section of this proposal, with 7.75% sales tax added. As a local firm, Western Scientific will waive delivery charges for this equipment. These will be purchased partly with $30,000 from a $50,000 CSRC supplies and equipment budget for the fiscal year beginning July 1, 2002. The balance of this purchase will draw on the requested NSF funds.

Matching funds: The $100,000 matching commitment from SDSU is composed of $70,000 in salary and benefits support to a dedicated CSRC System Administrator plus $30,000 in equipment funds towards the purchase of the Xfusion graphics workstations. The match in salary and benefits is equivalent to one quarter time or $23,333 over each of the three years of the grant period, less the stipulated maximum of 10% of the total equipment costs ($255,643). Funds will be provided by the College of Sciences at San Diego State University and will be available during the proposed project period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Andrew Cooksy**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Low-Coordinate Organometallics in the Gas Phase**

Source of Support: **NSF**
Total Award Amount: $ **1,805,927** Total Award Period Covered: **07/01/02 - 06/30/07**
Location of Project: **San Diego State University/University of Arizona**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **The University of Mississippi Connections Project**

Source of Support: **NSF**
Total Award Amount: $ **350,000** Total Award Period Covered: **08/15/99 - 07/31/02**
Location of Project: **University of Mississippi**
Person-Months Per Year Committed to the Project. Cal:**1.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Jose Castillo**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Pan-American Advanced Studies Institute Program (PASI) in Computational Science and Engineering University of Cordoba, Argentina, July 2002**

Source of Support: **National Science Foundation**

Total Award Amount: $ **100,000** Total Award Period Covered: **07/01/02 - 06/30/03**

Location of Project: **San Diego State University**

Person-Months Per Year Committed to the Project. Cal: **0.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

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*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **John Love**	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Protein Engineering: de-Novo Docking**

Source of Support: **Petroleum Research Fund**
Total Award Amount: $ **35,000** Total Award Period Covered: **09/01/02 - 08/31/04**
Location of Project: **San Diego State University**
Person-Months Per Year Committed to the Project. Cal:**6.00** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **A New Class of Anticancer Compounds for the Treatment of Ovarian Cancer**

Source of Support: **California Cancer Research Program**
Total Award Amount: $ **138,954** Total Award Period Covered: **06/01/00 - 05/31/03**
Location of Project: **San Diego State University**
Person-Months Per Year Committed to the Project. Cal:**3.00** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Protein Engineering: Novel Protein/Protein Docking By Design**

Source of Support: **San Diego State University Foundation**
Total Award Amount: $ **4,000** Total Award Period Covered: **01/01/01 - 05/31/02**
Location of Project: **San Diego State University**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Computer Assisted Protein-Based Drug Design**

Source of Support: **San Diego State University**
Total Award Amount: $ **5,000** Total Award Period Covered: **10/01/01 - 05/31/02**
Location of Project: **San Diego State University**
Person-Months Per Year Committed to the Project. Cal:**0.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Massimo Boninsegni**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **H2 Physisorption on Alkali Substrates**

Source of Support: **Petroleum Research Fund**

Total Award Amount: $ **60,000** Total Award Period Covered: **08/01/01 - 07/31/03**

Location of Project: **SDSU**

Person-Months Per Year Committed to the Project. Cal: **3.00** Acad: **0.00** Sumr: **0.00**

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Adsorption of Quantum Fluids Inside Carbon Nanotubes**

Source of Support: **NSF**

Total Award Amount: $ **150,000** Total Award Period Covered: **11/01/01 - 10/31/04**

Location of Project: **SDSU**

Person-Months Per Year Committed to the Project. Cal: **6.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:

Total Award Amount: $ Total Award Period Covered:

Location of Project:

Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Terrence Frey**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Structural Studies of Mitochondria**

Source of Support: **American Heart Association**
Total Award Amount: $ **60,000** Total Award Period Covered: **07/01/01 - 06/30/02**
Location of Project: **SDSU**
Person-Months Per Year Committed to the Project. Cal: **6.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Antonio Palacios**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: **Reduced Order Models of Heat Transfer in Fluidized Beds**

Source of Support: **Department of Energy**
Total Award Amount: $ **323,279** Total Award Period Covered: **09/01/00 - 08/31/03**
Location of Project: **SDSU**
Person-Months Per Year Committed to the Project. Cal: **6.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

Current and Pending Support

(See GPG Section II.D.8 for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: **Eric Sandquist**

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title: **Processing and Analysis of Images of Globular Star Clusters**

Source of Support: **NSF**
Total Award Amount: $ **170,588** Total Award Period Covered: **09/01/01 - 08/31/04**
Location of Project: **SDSU**
Person-Months Per Year Committed to the Project. Cal: **6.00** Acad: **0.00** Sumr: **0.00**

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Sumr:

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support

Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.

SDSU
Dept. of Chemical Sciences
RM 310
Attn. Andy Cooksy

Andy:

Thank you for your interest in Western Scientific! Enclosed is the price quotation, you requested. The quote includes installation and initial local set-up at no extra charge. For the first ninety days, tech support, parts and labor are free and local! After that, the parts and labor are TWO years on all equipment. We prefer on larger clusters to use terminal servers instead of KVM switches. They are more versatile, and you can remotely log in to a particular node.

Master Kilo Cluster Node	**UNIT**	**TOTAL**
QTY 1		
WX541-40RM, 1U-Master Node Unit	$ 2,490.	$2,490.
To Include:		
-1U single board node chassis w/4 ballbearing cooling fans		
-300W power factor correction power supply		
-(2) Pentium III 1.13Ghz Tualatin Processors		
-(1) Tyan 2518 Dual processor Server Mb.		
-1.0Gb-PC133 SD Ram		
-Low Profile floppy-cd drives		
-(2) Intel Pro **DUAL** 10/100 ports (Intel 82559, compatible w/ new 82543gc chipset)		
-Red Hat Linux		
-Video, Serial-KB interface on the motherboard.		
- (2) 100.Gb. AT/IDE Hard Drives		
TWO Year Warranty		
QTY 53		
WX541-18RM, 1U-Mini Cluster System	$1,765.	$93,545.
To Include:		
-1U single board node chassis w/ 4 ballbearing cooling fans		
-300 Watt power factor correction power supply		
-(2) Pentium III 1.13Ghz Tualatin Processors		
-(1) Dual processor Tyan 2518 motherboards w/ Via Chipset and 133Mhz front side bus.		
-1.0Gb-PC133 SD Ram		
- IBM 60Gb. IDE/AT Drive		
-(2) Intel Pro 10/100 Fe Controllers(Intel82559) per motherboard.		

-Red Hat Linux
-Video, Serial-KB interface on the motherboard.
TWO Year Warranty

TERMINAL SERVER

QTY 2		
Lantronix ETS32PR, 32 port terminal server	$2,450.	$4,900.

UPS

QTY 2		
APC Smart UPS 3003u w/ Linux Software	$1,550.	$3,100.
One Year Warranty		

CABINET

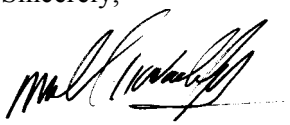
QTY 2		
WSCI -001, 77"-40U-NODE Usable Cabinet W Door	$2,450.	$ 4,900.
	TOTAL	**$108,935.**

OPTIONS:

WX5443, 1.1Tb Usable Raid	$26,750.
INCLUDES:	
Rackmount Fibre Channel Head unit includes:	
4u Rackmount system, W/ 512 Cache	
Dual Active/ Active Raid Controller(Fibre)	
No Single Point of Failure	
(8) Seagate ST118766LC 181.4Gb SCA SCSI Drives, 6+1+1	
Emulex PCI Fibre HBA(Requires 2U Master Node)	
Rackmount Enclosure	
128Mb Cache	
5 Yr. Warranty on Raid	
Sony 17' Flatscreen Monitor	$ 599.00
Onsite Service SDSU, 5x9x8hrs	$7000.00

Please allow two-three weeks for delivery. Quotation is good for 60 days. Thank you for the opportunity to quote!

Sincerely,



Mike Woodruff
Senior Sales Engineer
858 565 6699 Ext 204

Andy:

Thank you for your interest in Western Scientific! Enclosed is the price quotation, you requested.

5447 Pentium 4 Based Visualization Server	Unit Price
To Include:	
Deskside Chassis Dual Redundant power supplies	$3,240.00
W/ ball bearing cooling fans	
-(1) Pentium 4, 2.0Ghz. Processor	
-(1) Intel P-4 Server mb.	
-1.0Gb-RD Ram	
-Viewsonic 15" Flat Panel Monitor	
-Low Profile floppy-cd drives	
-Intel Pro 10/100 Controller	
(Intel 82559, compatible w/ new 82543gc chipset)	
-Red Hat Linux	
-GeForceVideo, 3-D 32Mb.	
-Adaptec U160 SCSI W/ IBM 18.2Gb Hard Drive	
- Mouse-KB	
- TWO Year Warranty	

OPTION

Viewsonic/ Sony 17" Flat Panel Monitor	Add	$ 425.00

Please allow two weeks for delivery. Quotation is good for 60 days. Thank you for the opportunity to quote!

Sincerely,

Mike Woodruff
Senior Sales Engineer
858 565 6699 Ext 204

sgi

Date: 1/16/02
Effective Thru: 2/15/02

Quote Number: BK 1-8TRTE / 1
Status: Valid

To: Andy Cooksy
San Diego State University
5500 Camponile Drive
San Diego, CA 92182
Tel: (619) 594-5571

From: Beth Klemmensen
SGI
655 Lone Oak Drive, ms. CRI-EAG
Eagan, MN 55121
Tel (877) 783-4369 Fax (651) 683-7115
bethk@sgi.com

Row	Qty	Model Number	Description	Unit Price	Disc.	Total	Support
1.0	1		Octane2				
1.1	1	WT5-1P360V6-218	Octane2 V6 Graphics R12000A 360MHz/2MB cache, 256MB, 18GB 10,000 RPM System Disk, 21" Monitor	$17,495.00	33.00%	$11,721.65	$1,020.00
1.2	1	P-CDR40-EXT	External CD-ROM 40X	$695.00	33.00%	$465.65	
1.3	1	D-MON21A-NC	21" Flat Trinitron, Tilt-Swivel, Color Monitor for Octane and Octane2				
1.4	1	SC4-AWE-6.5	IRIX 6.5 Advanced Workstation Environment for Visualization Systems (O2, Octane2, Onyx 3000)	$300.00	33.00%	$201.00	
1.5	1	CBL-SCSI3/3-.75	SCSI3 to SCSI3 Cable (.75m)	$100.00	33.00%	$67.00	
1.6	2	DK-P5-001	Power Cord - USA, Canada				
1.7	1	KBB-US	Keyboard Kit- United States for O2, Octane and Octane2				
1.8	1	MO5-CD	CD-ROM Update Media requirement - For Support Only				$240.00
			Subtotal: Octane2			$12,455.30	
			Subtotal: FullCare 1Y Warranty Upgrade				$1,260.00

Note: Sales of Silicon Graphics Products are subject to SGI's standard terms and conditions (including NET 30 DAYS & FOB ORIGIN), or those of the applicable SGI contract as well as SGI's Year2000 compliance warranty. SGI objects to conflicting or additional terms and conditions. Sale will be taxed unless exemption number is provided. Prices quoted do not include taxes, special handling or packaging unless specified. To expedite your order, please issue your PO using the products and descriptions indicated above. When carrier other than 'SGI Carrier' is requested, shipping terms will be Freight Collect.
Partial Shipment: Unless otherwise stated on purchase order, customer agrees to accept and pay for partial shipment. Upgrades: Initial product shipment acceptance and payment is independent of upgrade delivery.

--- --- ---

****Flexible financing options available through SGI Solutions Finance-****
The leader in financing advanced technology.
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Undiscounted Total:	$19,850.00
Product Subtotal:	$12,455.30
Support Subtotal:	$1,260.00
Grand Total:	**$13,715.30**

Beth Klemmensen

Note: Sales of Silicon Graphics Products are subject to SGI's standard terms and conditions (including NET 30 DAYS & FOB ORIGIN), or those of the applicable SGI contract as well as SGI's Year2000 compliance warranty. SGI objects to conflicting or additional terms and conditions. Sale will be taxed unless exemption number is provided. Prices quoted do not include taxes, special handling or packaging unless specified. To expedite your order, please issue your PO using the products and descriptions indicated above. When carrier other than 'SGI Carrier' is requested, shipping terms will be Freight Collect.
Partial Shipment: Unless otherwise stated on purchase order, customer agrees to accept and pay for partial shipment. Upgrades: Initial product shipment acceptance and payment is independent of upgrade delivery.

--- --- ---

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College of Sciences
San Diego State University
5500 Campanile Drive
San Diego CA 92182-4610
TEL: 619-594-5142
FAX: 619-594-6381
E-mail: office@sciences.sdsu.edu

January 17, 2002

Office of Integrative Activities
Major Research Instrumentation Program
National Science Foundation
Room 1270
4201 Wilson Boulevard
Arlington, VA 22230

Dear Sir or Madam:

As an indication of our enthusiasm and support for Dr. Cooksy's proposal entitled "Computer Infrastructure for the SDSU Computational Science Research Center," the College of Sciences will commit a total of $100,000 as our institution's cost share for this project, distributed as follows:

- $30,000 in the first year of the grant (academic year 2002/2003) towards equipment purchases, and
- $70,000 in salary support over the three-year period of the grant (one full-time position with annual salary of $70,000 at one-third time).

Sincerely,

Thomas R. Scott

Thomas R. Scott, Dean
College of Sciences