

RHEOLOGY OF MATERIALS OF EARTH'S MANTLE: HIGH-END COMPUTATIONAL/VISUALIZATION RESEARCH AND EDUCATION

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PROJECT SUMMARY

This career development plan aims to systematically bridge the gap between computational and Earth materials sciences. It will use high-end parallel supercomputing and visualization to address one of the fundamental challenges related to Earth materials. The challenge is to understand the rheological properties of mantle materials at typical pressures and temperature conditions of deep interior, which are experimentally inaccessible. The proposed strategies are to:

- Develop a scalable parallel algorithm based on a multiscale first-principles quantum mechanics (QM)/classical molecular dynamics (MD) approach, which will enable large-scale atomistic simulations.
- Investigate deformation mechanisms and processes including different defect types (ionic vacancies, protons, dislocations and grain boundaries) in major mantle oxide and silicate minerals (e.g., Mg-silicate perovskite, the predominant phase in the lower mantle).
- Apply/develop visualization techniques, including virtual reality type, to gain insight into the resulting massive multivariate datasets.

The results will furnish crucial information required for understanding the major geodynamical issues related to mantle rheology: 1) the radial and lateral variation of rheological properties, 2) the interaction of rheological behavior with water content and phase transformations, and 3) the relationship between the seismic anisotropy and the mantle flow pattern.

The proposed interdisciplinary research activities will be integrated into teaching/learning/training activities, which are to:

- Train a new generation of students with expertise in computational and Earth materials sciences through a dual-degree program (with a Ph.D. in computer science and an M.S. in Earth science)
- Develop an Access Grid-based remote teaching/learning environment (encompassing minority institutions in Louisiana).
- Co-organize computational science workshop for underrepresented groups and Mardi Gras conference which have previously been held at Louisiana State University (LSU).

The research and education plans are firmly based on the PI's prior accomplishments. The PI has previously contributed significantly to understanding single-crystal properties (structure, phase equilibria, lattice dynamics and elasticity) of major mantle materials. This project will take his initiatives to the next level, which will deal geophysically more relevant but challenging problems related to mechanical properties of polycrystalline minerals. The PI will have local access to sufficient resources to support the proposed projects, which include the world-class 1024-processor Linux cluster, ImmersaDesk virtual reality and Access Grid facilities recently acquired by LSU of which the PI is one of the full-scale users. He has recently developed/taught an interdisciplinary graduate course in scientific visualization. He has previously successfully co-organized above mentioned workshop and conference. The proposed project will make an extensive collaboration at national level.

§1. OBJECTIVES

The goal of this career development project is to establish an integrated interdisciplinary research and education at the interface of Earth science and information technology. There is an urgent need to systematically bring ideas of computer and materials sciences to significant problems in theoretical investigation of fundamental issues of Earth's materials. One such issue is to develop a firm theoretical basis to understanding the rheological properties of mantle materials at typical pressure and temperature conditions of deep interior that are crucial in gaining insight into the complicated dynamics of Earth's mantle implied by seismological observations and other sources (Fig. 1). Experimentally characterizing these properties under extreme conditions poses a tremendous challenge: For instance, no deformation experiments have yet been performed at mantle conditions for Mg-silicate perovskite, the predominant phase of the lower mantle – the single largest region of the Earth's interior. The different mechanisms (diffusion or dislocation creep) by which the mantle may deform in the solid state follow profoundly different pictures of mantle dynamics. Whether lattice preferred orientations that could be the sources of the seismic anisotropy relating to mantle flow may develop or not depend on deformation mode.

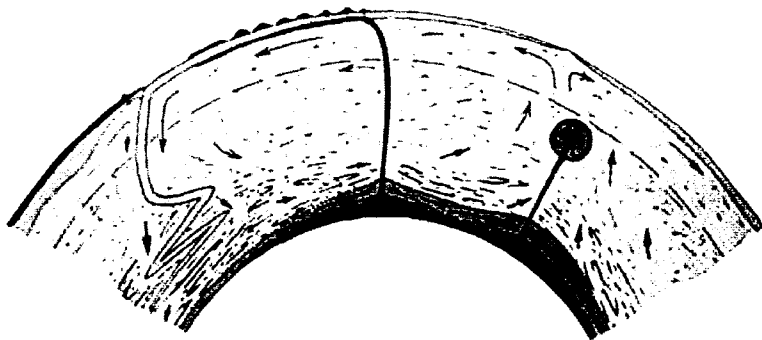


Fig 1. Mantle dynamics showing mantle circulations, subducts, plumes and tectonic plates

Studying rheological properties of mantle minerals theoretically represents an interesting, rich and challenging problem. Large multiscale simulations will be performed on massively parallel supercomputers to address the above issues. The simulations will predict the relevant materials properties under the pressure and temperature conditions that are experimentally inaccessible. They will bridge diverse length- and time-scales that are important in rheological processes. The specific objectives are to:

- Develop a multiscale approach that combines quantum mechanical (QM) calculations based on density functional theory (DFT) and classical atomistic simulations based on molecular dynamics (MD). A scalable algorithm will be designed to implement the hybrid QM/MD method on massively parallel machines such as a 1024-processor Linux cluster of LSU.
- Investigate deformation mechanisms in major mantle silicate and oxide phases including Mg-silicate perovskite at prevailing pressures and temperatures by computing
 - Energetics of ionic vacancies, protons, dislocations, and grain boundaries as well as their dependence on grain size.
 - Kinetics of defect migrations: vacancy hopping, proton motion, and dislocation glide/climb.
 - Dynamics simulations of deformations (diffusion/dislocation processes and resulting fabrics) of polycrystalline mineral phases under external anisotropic stresses (e.g., shear stresses which are most relevant in the boundary layers).
- Develop/apply graphical user interface (GUI) for visualization, including immersive and interactive virtual reality type, of the resulting massive multivariate datasets to gain insight into complex mechanical behavior of minerals.

The proposed interdisciplinary research activities will be integrated into teaching/learning/training activities. These will make broad substantive involvement of students and faculty including those from underrepresented groups. The specific objectives are to:

- Establish a dual-degree curriculum leading to a Ph.D. in computer science and an M.S. in Earth science. This will address the critical need of training a new generation of students with expertise in both disciplines. This will be an expansion of the existing dual-degree program (in computer science and physics) of the Department of Computer Science at LSU. To the best of our knowledge, an interdisciplinary dual-degree program coupling computer and Earth sciences does not exist in an academic setting.
- Develop an Access Grid-based remote teaching/learning environment. Access Grid is an ensemble of resources including multimedia equipments with interfaces to the Grid middleware, which allows group-to-group interactions through the Grid. Courses will be offered on the Grid

to students at minority institutions in Louisiana (Southern University in Baton Rouge, Southern University in New Orleans and University of Louisiana at Monroe). Selected undergraduate students will do summer internships in Earth materials research. This will be an opportunity for students to explore what impacts high-performance computing and visualization have on Earth science. This will also help in recruiting underrepresented students in the proposed dual-degree program.

- Co-organize the computational science workshop for underrepresented groups in which the participants will have hands-on training in building a PC cluster and performing parallel computations including MD simulation on simple mineral. A visualization component will be added to the workshop theme. This annual workshop was initiated in 2002.
- Co-organize the well-established Mardi Gras international conference, which has already been held at LSU for the last several years. The conference will bring together prominent computational and experimental scientists including those working in mineral physics and Earth science.

The proposed project is fundamentally about building intellectual collaborations between institutions – University of Southern California (Nakano, Kalia and Vashishta), University of Minnesota (R. Wentzcovitch), University of Michigan (L. Stixrude), and Southern University in Baton Rouge (Zhao and Khosravi) – and between disciplines – computer, materials and Earth sciences. A part of the output of the proposed project will be simulation and visualization tools, which will be disseminated through collaborations and a wave portal to enhance the computing infrastructure. Besides publication in the usual scientific journals, results will be presented at major AGU, MRS, APS conferences and Mardi Gras conference.

§2. GEODYNAMIC ISSUES IN RHEOLOGY

Seismic tomographic observations and other sources have implied the existence of large-scale circulation within the Earth's mantle but the geometry of the mantle flow appears to be highly complicated, particularly, in the vicinity of the boundary layers (transition zone and D" region) [e.g., *van der Hilst et al.*, 1997; *Kellogg et al.*, 1999; *Master et al.*, 2000]. Rheology is a key factor, which has strong influence on mantle convection and associated mass transport [e.g., *Karato et al.*, 2001]. It also affects the geochemical evolution because the nature of stirring of different chemical reservoirs depends critically on rheological contrast of mixing materials [e.g., *Manga*, 1996]. A number of fundamental issues related to mantle rheology remain unaddressed:

- Radial variation (depth-wise) of rheology: How does the strength of the lower mantle compare with that of the upper mantle and transition zone?
- Lateral (at constant depth) variation of rheology: How is rheology affected by phase transformations of component minerals, for example, in the subducted slabs? How is it affected by water content of the mantle?
- Relating seismic anisotropy observed in different portions of the mantle to the flow pattern: Does mantle deform so as to induce microstructures such as lattice-preferred orientation?

Two important sources to probe mantle rheology are: 1) experimental/theoretical data on rheological properties of relevant mantle minerals [e.g., *Meade and Jeanloz*, 1998; *Meade et al.*, 1995; *Merkel et al.*, 2002], and 2) geodynamic data such as post-glacial crustal rebound and gravity anomalies [e.g., *Mitrovica and Forte*, 1997; *Peltier*, 1998].

Any rheological variations and interactions in the mantle are presumably governed by rheological (i.e., mechanical) response of the materials that make up this region to the pressure, temperature and stress over geological time scales. However, knowledge about rheological properties of the component materials is still limited despite the significant progresses in deformation experiments in recent years. Deformation mechanisms (in particular, the easiest glide planes) are known in the dominant minerals, olivine and pyroxene, of the upper mantle [*Nicolas and Christensen*, 1987]. Past deformation experiments have been carried out on Mg-rich silicate perovskite with texture analysis made only on quenched samples from high pressure and 300 K [*Meade et al.*, 1995]. But very recently the shear deformation experiments have been performed to investigate deformation mechanisms and shear strength in situ of (Mg, Fe)O up to 47 GPa and 300 K [*Merkel et al.*, 2002] and those of perovskite up to 32 GPa and 300 K [*Merkel et al.*, 2003].

An alternative approach based on atomistic simulations, ranging from empirical to first-principles in nature, has proven to be a powerful addition to explorations of a wide range of properties of Earth materials. This approach will not only predict quantitatively different properties of the mantle materials but will also elucidate atomistic description of these properties. In particular, the first principles quantum mechanical (QM) calculations with their high predictive power have supplied in the last decade a huge

amount of critical information including, that which is difficult to measure and/or yet to be measured experimentally at extreme conditions of geophysical relevance. To the date, these calculations have mostly addressed the single-crystal properties of major mantle materials such as crystal structure, phase transformations, electronic structure, vibrational spectra, thermodynamics, and elasticity [e.g., *Stixrude and Cohen*, 1993; *Wentzcovitch et al.*, 1993; *Karki et al.*, 1997; 1999; a review by *Karki et al.*, 2001; *Oganov et al.*, 2002; *Karki et al.*, 2002; 2003]. There is a need of extending the QM calculations to deal with geophysically more relevant rheological problems of important mantle materials.

§3. CHALLENGES IN COMPUTATIONAL MINERAL RHEOLOGY

A key challenge is to understand the essential physics of rheology of mantle minerals in the deep Earth conditions that is a prerequisite for realistic geodynamic models. It is important to note that deformation in solids does not take place homogeneously. Experimental observations on minerals have shown that crystal defects play an important role: A mineral without defects would be too strong to deform or diffuse. The presence of crystal defects causes an increase in the local internal stress in their vicinities. As a result, the application of a small external stress may be enough to mobilize a defect (i.e., easy to cause bond breaking/reconstruction near defect core), resulting in dislocation or diffusion creep. Understanding mechanical properties of a mineral thus requires quantitative characterization of active point (vacancies, interstitials, protons) and extended (dislocations, grain boundaries) defects in it. Dynamics simulations of polycrystalline minerals deformed under anisotropic stresses are needed to predict and elucidate deformation mechanisms (diffusion or dislocation creep) and resulting fabrics that are active in the deep mantle. Very little work has been done in this direction, including first-principles calculations of point defects in forsterite [*Brodholt*, 1997; *Brodholt and Refson*, 2000], defect energetics in MgO [*Vita et al.*, 1992] and ionic-model based calculations of chemical diffusivity in MgO [*Ita and Cohen*, 1997].

Studying rheological properties of minerals is computationally a very challenging problem: The difficulty arises from the wide range of length and time scales at which the various processes occur during the deformation – ranging from the Angstrom and picosecond scales of the atomic processes (e.g., bond breaking/reconstruction), to beyond the millimeter and second scales of the long-range effects (e.g., macroscopic deformation fabrics). This clearly means that very different models are needed to deal with phenomena at so different scales. From the point of view of atomistic modeling, it is now possible to handle system sizes in nanometer range and time scales of up to several nanoseconds.

First-principles approach is at present feasible with systems containing up to 10^5 atoms [*Shimojo et al.*, 2001]. This means that even a nanocrystalline mineral is still fully not within the reach of quantum mechanics. On the other hand, atomistic simulations based on empirical potential molecular dynamics (MD) can be applied to problems where the natural length scale is in the nanometer range (up to 10^{10} atoms) [*Nakano et al.*, 2001]. The effects of the defects in the regions around them where local electronic structures are important need to be treated quantum mechanically. The interatomic interactions in such regions must be calculated from first principles to describe bond breaking/reconstruction accurately. The outer regions, however, can be simulated with classical MD to understand long-range mechanical phenomena. This naturally calls for a multiscale approach where the realism of the simulation progressively decreases with distance from the defect cores in favor of computational efficiency [e.g., *Eichinger et al.*, 1999; *Ogata et al.*, 2002]. Fully first-principles QM and/or hybrid multi-scale QM/MD large-scale simulations proposed in this project will play a major role in the next generation of computational research on Earth materials.

Because the time scale of dynamics simulation is set by atomic motion, only very short periods of time can be sampled during the simulation. Typical simulation times are in the nanosecond range. These time scales are far shorter than geological time scales over which mantle minerals might have deformed. The creep rates in nature (e.g., 10^{-12} s⁻¹) are many orders of magnitude slower than the slowest strain rates accessible in deformation experiments (10^{-8} s⁻¹) and simulations (10^6 s⁻¹). Nevertheless, static calculations of defect energetics and kinetics (in which time-scale is irrelevant) and atomistic dynamics simulations of deformations under anisotropic stresses (performed at high strain rates) will contribute to better reveal the fundamental physics of the rheology of mantle minerals at high pressures and high temperatures, and hence that of the rheology of the mantle itself.

Gaining insight into massive datasets produced by simulations for important information on various properties and processes of mantle minerals poses a tremendous challenge. The datasets in general are time-dependent (dynamic), irregular and multivariate. Scientific visualization particularly in an immersive and interactive virtual reality environment provides an efficient-effective solution through the identification of small- to large-scale patterns and other features of a display [e.g., *Asish et al.*, 2002]. It also allows us to visualize a simulated system to evaluate the model that is used and to monitor

simulation while it is being performed interactively, a process called computational steering. Two major issues in visualization are representation and interaction. First is how to render the data such as simultaneous display of multiple variables or properties using the advanced three-dimensional (including stereographic) computer graphics. Second is how to interact with the system to explore the data from different prospects. Different rendering techniques are often needed for different specific purposes such as rapid navigation through the data, emphasis on data features, realistic rendering of data.

§4. RESEARCH PLAN

§4.1 RHEOLOGY OF SILICATES AND OXIDES

Various crucial rheology-related properties and processes in major mantle silicates (Mg-silicate perovskite, wadsleyite, spinel, Ca-silicate perovskite) and oxides (MgO, SiO₂, CaO) will be investigated in a quantitative manner at high pressures and temperatures. These include point and extended defects, associated diffusion/dislocation creep and long-range phenomena, deformations of polycrystals under anisotropic stresses.

Point defects such as vacancies, protons, interstitials (Fig. 2a) play an important role in various physical properties of minerals including diffusion, creep, electrical conduction, and seismic attenuation. The distorted crystal lattice around defects provides rapid diffusion pathways within crystals; diffusion most commonly occurs by a vacancy-hopping mechanism, whereby ions jump into neighboring vacancies. Under certain conditions, the dominant deformation mechanism may be diffusion creep or diffusion-controlled dislocation climb. A related issue is the water content of minerals, which has been observed to have profound effects on mineral properties: The trace amounts of water make minerals weaker and enhance diffusion rates dramatically in them. The water content can be treated in the form of H defects (i.e., protons). Many silicate minerals in the mantle are known/believed to accommodate significant amounts of water into their structures [e.g., *Bell and Rossman, 1992; Kohn, 1997*]. Some theoretical studies of mineral-water interactions were previously carried out for forsterite and olivine [*Wright and Catlow, 1994; Haiber et al., 1997; Brodholt and Refson, 2000*]. Several questions regarding the point defects in mantle minerals remain unanswered: What are energetically favorable vacancy sites for different atom types (Mg, Si or O)? What are their concentrations? How are protons incorporated into a given mineral structure? What are diffusion mechanisms and rates for different defect types including protonic defects? What are the long-range mechanical phenomena (e.g., deformation fabrics) associated with these defects? All these issues need to be addressed for major silicate and oxide minerals at geophysically relevant conditions.

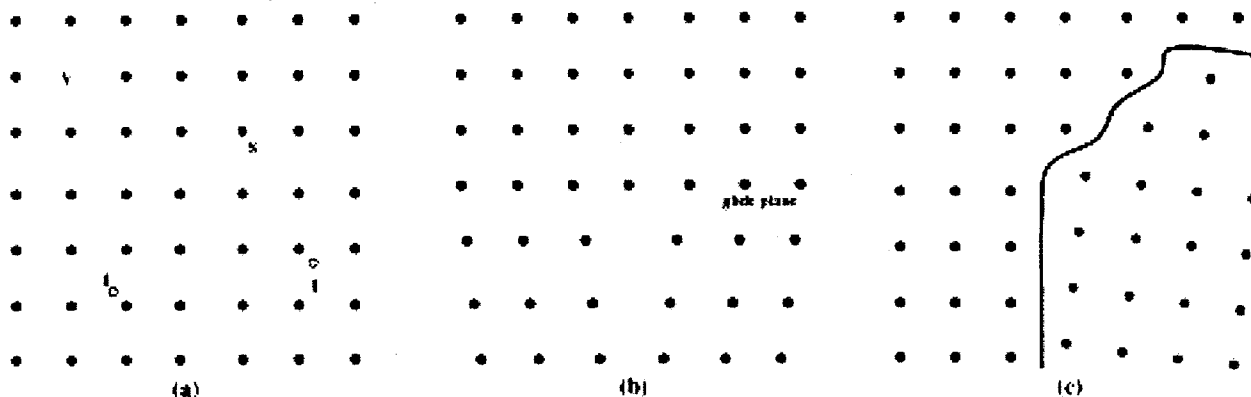


Fig. 2: a) Point defects (V: vacancy, S: substitutional impurity (proton), I: interstitials (self or impurity)); b) Dislocation (edge); c) Grain boundary.

The extended defects such as dislocations (Fig. 2b) provide a driving force for deformation process and their movement can lead to the formation of crystallographic preferred orientations. Two types of dislocation movement (called dislocation glide or slip) are relevant for plastic deformation: First, edge dislocation movement results in part of the crystal moving perpendicular to the dislocation line, and second, screw dislocation edge movement results in part of the crystal moving parallel to the dislocation line. A slip system is defined by the plane (i.e., the glide plane) in which dislocation moves and direction (i.e., the glide direction) in which it moves. Every mineral has some favorable (dominant) slip system, which is sensitive to the applied stress levels, as well as to the confining pressure and temperature.

A critical shear stress as resolved onto the slip plane in the slip direction is needed to cause dislocation motion, i.e., break shortest bonds. Dislocations can also act as fast diffusion pathways: Climb is a diffusive process whereby the dislocation line moves perpendicular to the dislocation line direction, but within the plane of the extra half-plane of atoms. The following questions are yet to be answered for majority mantle materials at geophysically relevant conditions: What is the nature of dislocation process (glide versus climb)? What are the dominant slip systems (the easiest glide planes) and the associated critical shear stresses? How does the nature of slip system change with pressure and temperature? What are the long-range mechanical phenomena (e.g., deformation fabrics) associated with different dislocations?

Dislocations or point defects are thus the carriers for deformation/diffusion in crystalline materials and depending on the nature of interface between grains (Fig. 2c) they can travel across them or not. Grain-boundaries and grain-size are two important variables in this respect: High-energy grain boundaries act as barriers for defect migration, and as a result, defects generated inside a grain repel each other. This mutual interaction together with external applied stress causes defects to concentrate in the vicinity of the boundaries. When the stress field resulting from the addition of individual defect contributions reaches some critical value, it activates sources in neighboring grains. At the smallest grain sizes, extended dislocation sources inside grains can hardly exist because size and image force limitations; only dislocation emitted from a boundary can eventually travel across the grain. It is possible that a competition between dislocation-dominated (glide/climb) and grain-boundary-dominated (sliding) processes occurs with varying grain size. What is the nature of the competition? What are the stable interfaces (boundaries) between grains? How does the grain-size affect deformation mechanisms and resulting fabrics? How does the strength (yield stress) of a polycrystalline mineral vary with pressure and temperature? Such studies were previously carried out on nanophase metals using molecular dynamics simulations [e.g., Swygenhoven *et al.*, 1999; Schiotz *et al.*, 1999; Yamakov *et al.*, 2002].

Proposed Research: We will perform the following investigations:

- *Energetics of defect emission including ionic vacancies, protons, dislocations and grain boundaries:* The structure containing a given defect (point or extended type) will be fully optimized and its energy relative to the perfect crystal (i.e., a defect-free crystal) will be calculated quantum mechanically whenever possible. Vacancies will be considered at all nonequivalent sites for each atom type; for example, perovskite has two nonequivalent O sites (O1 and O2). Several possible ways of incorporating protons including their binding at cation and silicon vacancies as well as at interstitial sites will be explored. Different dislocations will be generated choosing their glide planes along different crystallographic planes including those with the maximum atomic density and studied. Grain boundaries for low- to high-angle misorientations between neighboring crystals will be studied to better characterize stable interfaces between grains. Calculated energetic differences between defects of a given type will give an idea about relative concentrations of these defects because defect concentration is exponentially inversely dependent on defect energy. For instance, the concentration ratio of two similar defects differing on sites or glide planes can be expressed as $n_2/n_1 = \exp(-\Delta E/kT)$, where ΔE is the emission energy difference and n is the number of defects.
- *Kinetics of defect migration including vacancy hopping, proton motion, and dislocation glide/climb:* The activation energies will be calculated along the migration paths of different defects. Only paths constrained by symmetry will be considered for both point defects and dislocations. The calculated kinetics and energetics will help predict the favorable vacancy- and proton-sites, and dominant glide planes. The calculated height and shape of the energy barriers as well as the jump geometry (i.e., the path of a migrating ion or dislocation) will be used to quantify diffusion/dislocation rates.
- *Atomistic characterization of deformation mechanisms:* Atomistic dynamics of a given nanocrystalline mineral containing single to multiple defects (point or dislocation) under deformation will be simulated over time periods of several nanoseconds. This will provide the local structure around the defect cores as well as long-range mechanical phenomena (stress and strain distributions) associated with the defects in the nanocrystal. The defect cores will be explicitly treated with quantum mechanics whereas the surrounding region with classical molecular dynamics (see section 4.2: Computational Techniques). On the other hand, the investigation of intra- and inter-granular diffusion and dislocation, and grain boundaries processes will involve polycrystalline systems. The grains will be produced using Voronoi construction: A set of grain centers are chosen at random, and the part of space closer to a given center than to any other center is filled with atoms in a randomly rotated crystal lattice of the symmetry of the material studied. This will generate a grain-size distribution close to a log-

normal distribution. The grain boundaries will be relaxed by removing atoms that are too close and by annealing before deforming the polycrystal. Deformation of polycrystalline minerals containing a few hundred grains (a few nm in sizes) with random grain boundaries in an anisotropic stress field will be simulated. The above dynamics simulations will be performed at different strain rates and for different grain-sizes. Due to very large number of atoms in a polycrystalline system, these simulations will be performed using the hybrid QM/MD multiscale or simply classical MD methods (see section 4.2: Computational Techniques).

Prior Accomplishments: The proposed research plan will take the computational studies the PI has been pioneering over the last several years to the next level, which is crucial to better understanding of mantle rheology and dynamics. Since the beginning of the graduate work, the PI has extensively applied density functional theory in first-principles calculations on important Earth materials at geophysically relevant pressure and temperature conditions. These studies have substantially contributed to an exploration of the foundation of materials behavior in the relationship between structure, bonding, and composition under pressure and temperature. He has previously calculated the

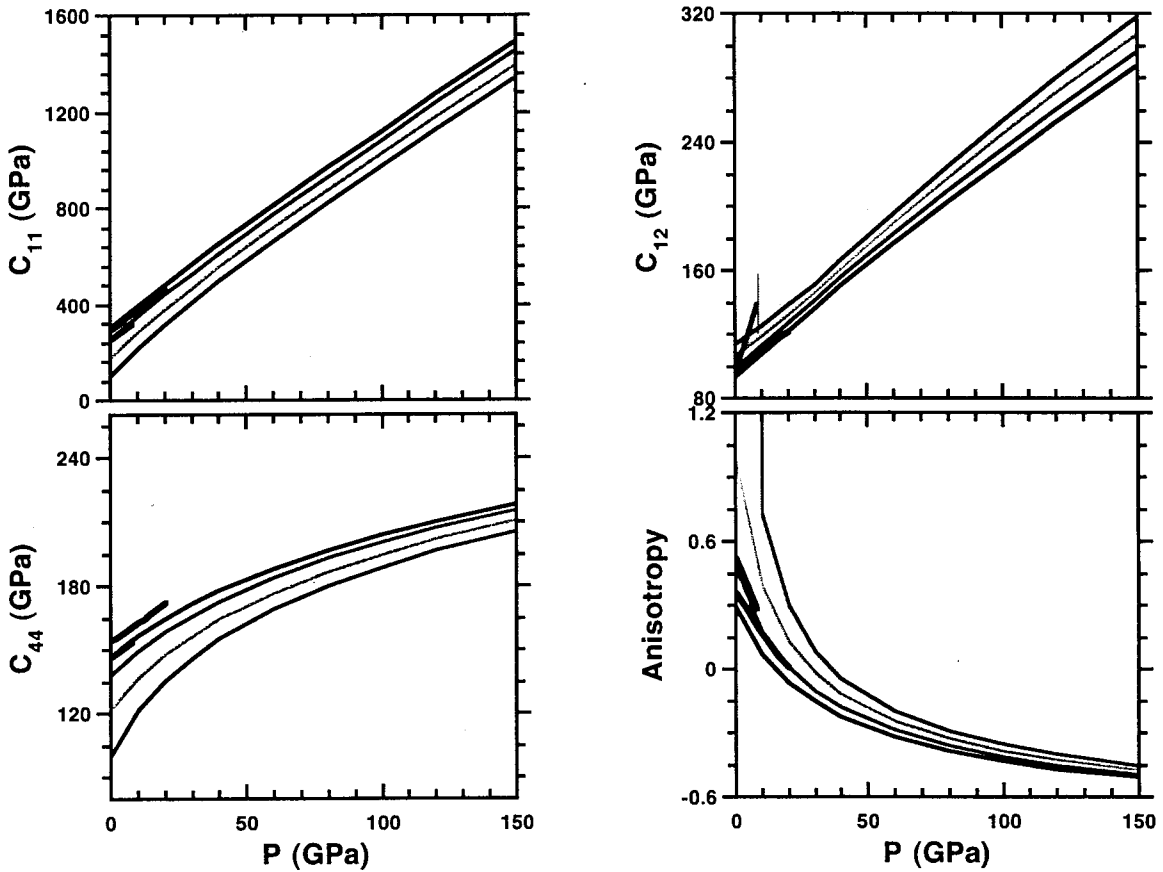


Fig. 3: Calculated elastic constants and anisotropy of MgO as a function of pressure along isotherms, 300 K (black), 1000 K (red), 2000 K (green), and 3000 K (blue) [Karki *et al.*, *Science*, 2000]. Experimental data are at 300 K (black) and 800 K (red) [Chen *et al.*, 1998; Sinogeikin and Bass, 1999].

structural parameters, vibrational frequencies and athermal elastic coefficient tensor (c_{ij}) of several silicate and oxide materials throughout the mantle pressure regime (0 to 136 GPa) [a review by Karki *et al.*, 2001 and references therein]. The effects of pressure on the calculated properties have been shown to be dramatic. For instance, the elastic constants increase by as much as a factor of five over the pressure regime of the Earth's mantle. Moreover, the effect is not uniform among different elastic

constants. An important consequence of this is that not only the magnitude but also the nature of the elastic anisotropy change significantly with pressure [Karki *et al.*, 1997a; 1997b; 2001].

Although the effects of pressure are by far the predominant one, the effects of temperature are not negligible. The PI has extensively studied the temperature-dependent properties of Earth materials. He has performed a benchmark calculation on MgO to determine its c_{ij} at high pressure and temperature (Fig. 3) using the lattice dynamics method that exploits the volume and strain dependencies of vibrational frequencies within the quasi-harmonic approximation to determine the thermal contribution to the free energy [Karki *et al.*, 1999, 2000]. The required bulk phonon dispersions were calculated from linear electronic response calculations with density functional perturbation theory. More recently, The PI has extended these calculations to study the thermal equations of state and elastic constants of MgSiO₃ in its perovskite and ilmenite phases [Karki *et al.*, 2001, 2002, 2003; Wentzcovitch *et al.*, 2003].

These results on component minerals at geophysically relevant conditions have allowed us, for the first time, to test mantle compositional models by directly comparing the predicted longitudinal and shear wave isotropic velocities of various silicates and oxides with corresponding seismic profiles, see Fig. 4 [Karki and Stixrude, 1999; Karki *et al.*, 2001; Wentzcovitch *et al.*, 2003]. A recent comparison of the calculated wave velocities of aggregates of MgO and MgSiO₃ perovskite over the entire lower mantle pressure and temperature regime with the seismic velocity profiles has given an indication of super-adibaticity and/or heterogeneity in the bottom half of the lower mantle [Karki *et al.*, 2001; Wentzcovitch *et al.*, 2003]. Significant mineralogical contributions to the observed lateral heterogeneities in wave velocities in the deep mantle could be associated with the lateral thermal anomalies [Karki *et al.*, 2001; Karato and Karki, 2001]. Also, these studies have shown that pressure suppresses the temperature effects on the elastic anisotropy of MgO and MgSiO₃ perovskite thereby making them highly anisotropic towards the bottom of the lower mantle [Karki *et al.*, 1999; 2000; Wentzcovitch *et al.*, 2003].

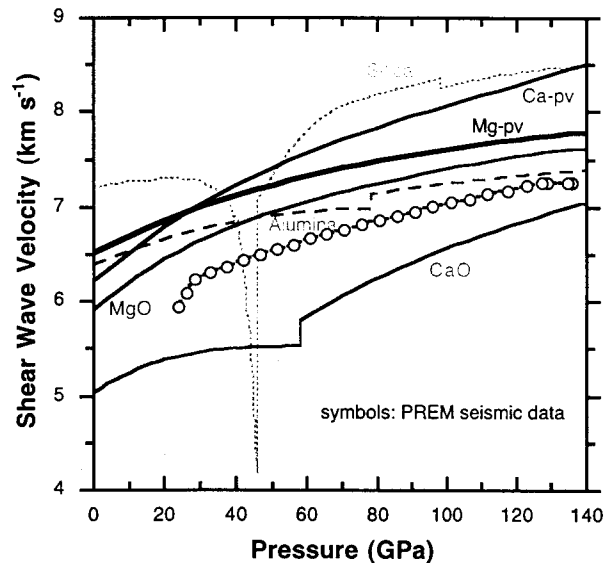


Fig. 4: Comparison of the calculated shear wave velocities of component minerals [Karki *et al.*, 2001] with the seismic data from Preliminary Reference Earth Model

§4.2 COMPUTATIONAL TECHNIQUES

The proposed computational studies of rheology of mantle materials will exploit three techniques: 1) first principles quantum mechanics (QM), 2) classical molecular dynamics (MD), and 3) a hybrid QM/MD multiscale scheme. The application requires little or no modification of their existing parallel implementation to development of new scalable parallel algorithms, depending on the needs posed by specific problems or sub-problems of interest.

QUANTUM MECHANICAL (QM) ALGORITHM: The density functional theory (DFT) [Hohenberg and Kohn, 1964; Kohn and Sham, 1965] has already proven to be an important contributor to our understanding of Earth materials at extreme conditions. The DFT is, in principle, an exact theory of the ground state and it maps an interacting many-electrons problem to N single-electron problems. In the Kohn-Sham (KS) formulation, the single-electron problem can be expressed as

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V_{I-E}(\vec{r}) + V_H(\vec{r}, \rho(\vec{r})) + V_{XC}(\vec{r}, \rho(\vec{r})) \right] \psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r}) \quad (1)$$

where V_{I-E} is the pseudopotential for valence electrons; V_H is the Hartree potential; and V_{XC} is the exchange-correlation potential treated within local density or generalized gradient approximations. The charge density is given by $\rho(\vec{r}) = \sum_i |\psi_i(\vec{r})|^2$. The KS equation constitutes a self-consistent field problem, that is, the self-consistent solutions (electronic wave functions $\psi_i(\vec{r})$ and eigenvalues ϵ_i) can be

obtained by iteratively solving the KS equation. The total energy of a system of atoms located $\{\bar{R}_a\}$ can be computed as

$$E_{QM}(\{\bar{R}_a\}) = T[\rho] + E_{I-E}(\{\bar{R}_a\}, [\rho]) + E_H[\rho] + E_{XC}[\rho] + E_{I-I}(\{\bar{R}_a\}) \quad (2)$$

where E_{I-I} is the interaction energy between ion cores often calculated using Ewald summation.

The DFT has successfully been applied to the simulation of solids including those containing defects in different ways [Payne *et al.*, 1992]: In the *supercell approach*, a solid is approximated using a cell (or supercell) of atoms and the charge density expanded in a basis of plane waves. A given defect is placed in the supercell to emulate the solid-state environment. However, defect-defect interactions need to be minimized by using a sufficiently large cell or need to be corrected somehow [Leslie and Gillan, 1985]. On the other hand, in the *cluster approach*, a solid is approximated by a cluster of atoms and the charge density expanded in a basis of Gaussian functions. A defect is placed at the center of the cluster to emulate the solid-state environment. However, artificial surface effects need to be minimized by using a sufficiently large cluster and passivating dangling bonds at the cluster surfaces with H atoms. Both the approaches are applicable to point defects in minerals. But a better way to deal with extended defects (e.g., dislocations) is the *supercell-cluster hybrid approach* (Fig. 5). Here a dislocation is placed in a model, which is periodic along the dislocation line; however, it is non-periodic with H-terminated surface perpendicular to the line direction.

Proposed Research: The parallel DFT algorithm (which the PI has previously used extensively in the case of Earth materials) will be used to study point defects (including vacancies, interstitials and protons) within the supercell approach, and dislocations within the supercell-cluster hybrid approach. In particular, a series of static calculations of activation energies will be performed for different defect emission and migration. This algorithm, however, scales asymptotically as $O(N^3)$ so it becomes a bottleneck for systems containing more than a thousand atoms. Larger systems will be needed to deal with grain boundaries and grain size-effects. We will develop/apply the parallel linear-scaling ($O(N)$) DFT algorithm based on localized wave functions combined with a real-space multigrid approach (in collaboration with University of Southern California) [Mauri and Galli, 1994; Shimojo *et al.*, 2001]. This will enable DFT calculations on systems containing 10^3 - 10^5 atoms.

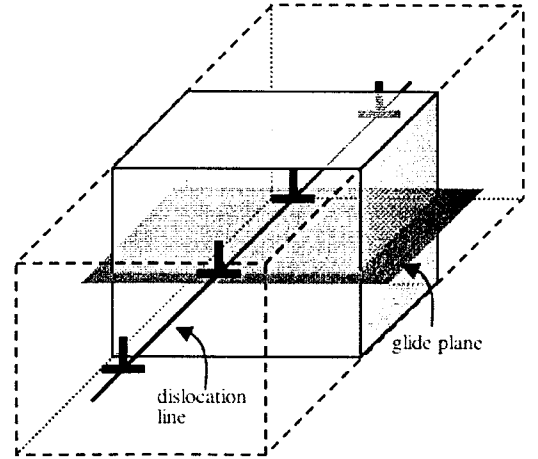


Fig. 5: A dislocation in a supercell-cluster hybrid model (cluster is shown as a box)

MOLECULAR DYNAMICS (MD) ALGORITHM: The MD approach uses empirical inter-atomic potentials, which are generally composed of two-body terms:

$$E_{MD}(\{\bar{R}_a\}) = \frac{1}{2} \sum_a m_a \bar{v}_a^2 + \frac{1}{2} \sum_{a,b} \phi_2(\bar{R}_a, \bar{R}_b) \quad (3)$$

but may also contain three-body terms. In MD, one obtains the phase-space trajectories (positions and velocities of all atoms at all time) by numerically integrating Newton's equations of motion, which are a set of differential equations [Allen and Tildesley, 1987]. Accurate interatomic potentials are essential for describing how atoms interact with each other in realistic simulations of materials [e.g., Matsui and Price, 1992; Choudhury *et al.*, 1998; Chaplot *et al.* 2000]. The MD method has widely been used to perform atomistic simulations of a wide range of physico-chemical properties of a variety of materials involving large systems (containing 10^8 - 10^{10} atoms), which at present cannot be simulated with any QM method.

Proposed Research: We will apply and further develop the parallel MD algorithm [which has recently been developed by the PI and co-workers] to study the material problems or sub-problems in which long-range mechanical effects (stress and strain distributions rather than local atomic processes) are of prime interest. Large-scale dynamics simulations of deformations of polycrystalline minerals (containing a few hundred nano-size grains) under anisotropic stresses (e.g., shear stresses) will be performed.

COUPLING QM WITH MD: The hybrid multiscale QM/MD approach has taken on an increased significance in recent years in dealing with large-size problems in which two different length-scales (atomic- and long-range) need to be treated differently [e.g., Eichinger *et al.*, 1999; Ogata *et al.*, 2002].

It essentially embeds a QM system described by real space-based DFT in a classical system of atoms interacting via an empirical interatomic potential. The method was previously applied to dynamic simulations of material processes such as oxidation of Si(111) surface and interaction of water molecule in Si crack coupled with long-range mechanical phenomena [Ogata *et al.*, 2002; Kikuchi *et al.*, 2002]. Handshake atoms are introduced to a couple the quantum and classical systems dynamically based on the scaled position method [e.g., Svensson *et al.*, 1996; Eichler *et al.*, 1996]. The hybrid method uses an additive hybridization approach based on a linear combination of QM and MD potential energies:

$$E = E_{MD}^{system} + E_{QM}^{cluster}(\{\bar{R}_{QM}\}, \{\bar{R}_{HS}\}) - E_{MD}^{cluster}(\{\bar{R}_{QM}\}, \{\bar{R}_{HS}\}), \quad (4)$$

where E_{MD}^{system} is the MD potential energy for the entire system and the last two terms represent the QM correction $E_{QM}^{cluster}$ is the QM total energy of an atomic cluster (its dangling bonds are terminated by H atoms to provide appropriate boundary conditions) and $E_{MD}^{cluster}$ is the MD potential energy of cluster (terminated by appropriate MD atoms). The hybrid QM/MD algorithm enables large-scale simulations involving $10^8 - 10^{10}$ atoms in which 10^2 to 10^4 atoms will be treated from first principles. As such, the multi-scale approach is useful for elucidating and quantifying – in a degree of detail not possible at present experimentally – the atomic-level description of material characteristics.

Proposed Research: We will develop/apply the hybrid QM/MD simulation algorithm on massively parallel computers. It consists of first dividing processors into the QM and MD calculations (task decomposition) and then using spatial decomposition in each task. The additive hybridization makes the QM and MD subtasks entirely independent except for the exchange of cluster-atom coordinates and calculated forces. Dynamic coupling between the QM cluster and surrounding MD system will be allowed to deal with defect emission and migration during simulations. Multiscale simulations will be performed to investigate the point and extended defects coupled with long-range mechanical phenomena in an extended system by treating the defect cores quantum mechanically and surrounding regions classically.

Prior Accomplishments: The PI has a longtime experience and expertise in quantum mechanical calculation of Earth materials problems by successfully working with different parallel DFT algorithms (PWSCF and CASTEP). He has developed algorithms to perform structural optimization under an anisotropic stress [Karki, 1999, unpublished] and derive thermo-dynamic and elastic properties of minerals [Karki *et al.*, 2000; 2001]. He has recently developed a massively parallel MD algorithm based on spatial decomposition and multiple time-step schemes and performed a million-atom simulation [Vemparala, Karki *et al.*, *Parallel Computing*, 2003, submitted]. The computation with this MD algorithm scales as N/P while communication scales as $(N/P)^{2/3}$ for an N -particle system and P -processors. Our scalability performance test shows that the program scales well up to 1024 processors on the LSU Linux cluster (Fig. 6).

§4.3 VISUALIZATION

Extracting useful information from massive simulations requires a visualization approach, which will allow users to visualize the dynamics of the constituent atoms with an option of displaying various attributes produced by simulations. *Atom Viewer* is a direct particle rendering visualization tool that has been implemented in a virtual reality environment allowing users to have a real-time walk through the large-scale (up to billion-atoms) simulations [Ashish *et al.*, 2002] (see Fig. 7). It represents atoms by

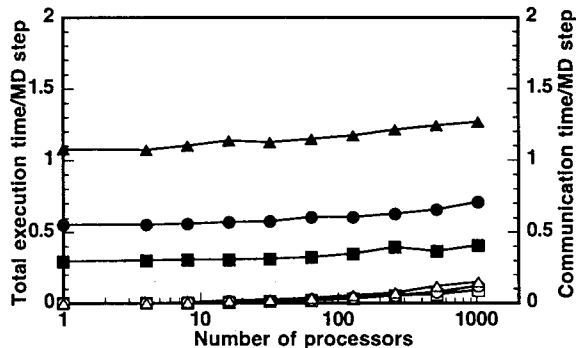


Fig. 6: Total execution time (solid symbols) and communication time (open symbols) as a function of P for different work loads: $N/P = 5280$ (squares), 10560 (circles) and 21120 (triangles).

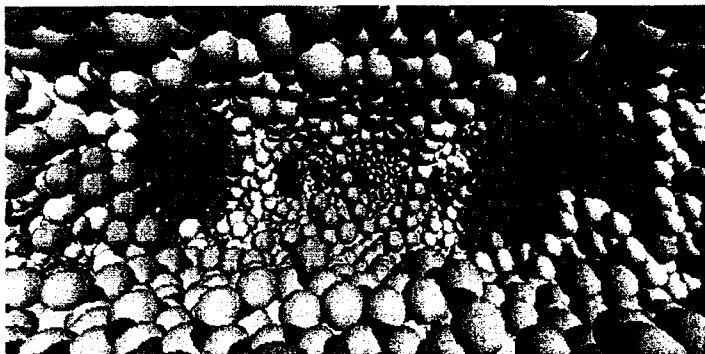


Fig 7: Visualization of fracture in SiN-matrix SiC-fiber composite

spheres and their attributes by appropriate color-coding. It achieves high rendering speed (number of frames per second) by using a parallel and distributed visibility-culling scheme to process data subset that lies within the field of view for a given viewing point.

Proposed Research: We will develop/apply immersive and interactive graphical user interfaces (GUI) with real-time visualization response to enhance the understanding of massive multivariate simulation datasets:

- *Atom Viewer* will be used to visualize the atomic configurations from simulations (in collaboration with University of Southern California). An *overview-and-details scheme* will be added. Only the details display window will show atomic-scale information (e.g., atomic bonding, charge transfer, atomic displacements) while the overview display window will show coarse-level information and overall variations of different properties.
- Different vector and tensor visualization tools will be developed to meet the specific visualization needs posed by simulations: Visualization of rheological datasets involves analysis of defect-core motions, and resulting stress and strain field. We will implement the standard techniques, namely glyphs and streamlines to visualize a vector field, and ellipsoids and hyper-stream-surfaces to visualize a tensor field using OpenGL graphics library [Woo *et al.*, 1999] and/or VTK (visualization toolkit). Some of these tools will finally be adopted in the virtual reality environment using CAVE library.

Prior Accomplishments: The PI has gained a substantial experience with *Atom Viewer*, which is

covered in his scientific visualization course. He has recently developed a GUI for the computed multivariate elasticity data for mantle minerals [Karki *et al.*, 2003, in preparation]. The scheme for visualizing the elastic anisotropy of a mineral in response to pressure and temperature, for instance, involves two steps: First, the wave equation is solved on an adaptive grid of propagation directions in three-dimensional space to get the wave velocities from elastic moduli. Second, the velocity distribution is displayed using polygon-surface technique and color-coding. Any distortion from the spherical shape, for instance, represents the anisotropy giving information on the fastest and slowest wave propagation. Fig. 8 demonstrates the GUI developed using OpenGL that allows us to explore how the velocity-direction surfaces for three elastic waves (one longitudinal and two shear) of MgO change as pressure is varied. This will be put in the ImmersaDesk where a three dimensional velocity-surface makes a true sense. Other on-going project includes visualization of vector data from computational fluid dynamics simulations (in collaboration with Iyengar and Acharya).

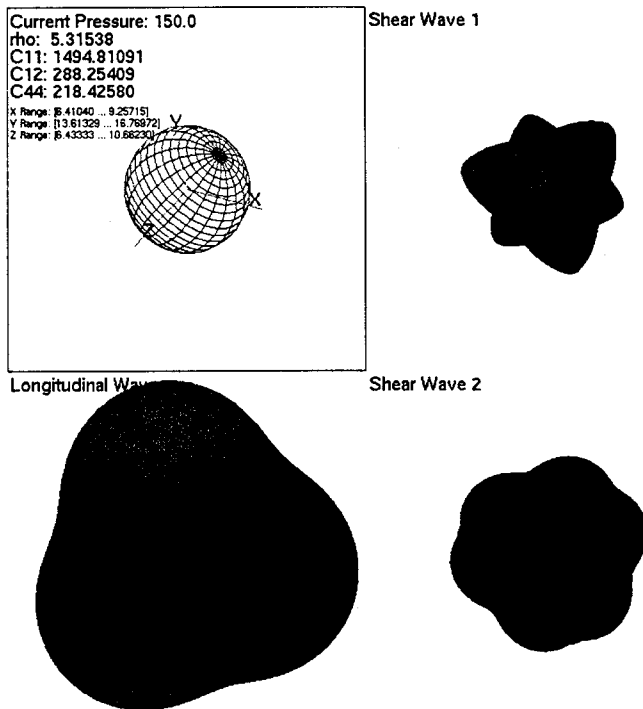


Fig 8. Visualization of wave velocity anisotropy of MgO at 150 GPa. Brightest region represents the maximum velocity and darkest region represents the minimum velocity for each wave.

§5. CHALLENGES IN EDUCATION AND TRAINING

The present and future trends in high-end computational research on forefronts of Earth materials imply a critical need of producing a new generation of scientists who will have expertise in both computational and Earth materials sciences. The proposed interdisciplinary research opens the possibility of developing its education counterpart. Such an endeavor is challenging: Computer and Earth sciences are two very different disciplines; each discipline has developed its own set of courses and resources. An efficient bridging mechanism is needed to systematically draw the disciplines into closer proximity.

Interactive learning environment will help students comprehend various phenomena (from atomic to geological scale) related to the Earth itself and its component materials. Use of visualization tools can be an effective approach in this context. Visualization is a process of displaying a given dataset or information or phenomenon with advanced three-dimensional computer graphics including an immersive and interactive environment in which users are completely blocked from the outside world. A laboratory equipped with visualization hardware and software will assist students to learn various phenomena related to the Earth's interior.

Louisiana is one of the states having large African-American communities. To enhance participation of underrepresented groups poses tremendous challenge: Only the resource or infrastructure development alone cannot be much helpful. These resources need to be used in an effective way to reach broader minority audiences. What is needed is the practical mechanism of actively involving groups traditionally underrepresented in computer and Earth sciences into research and training activities. Such initiatives should emphasize a combined involvement of minority students and their mentors at emerging areas of high-end computational research. Collaborative environment involving minority institutions should be enhanced.

§6. EDUCATION AND OUTREACH PLAN

The proposed research project will accomplish the maximum impact when the interdisciplinary research activities will be appropriately integrated into the interdisciplinary teaching/learning/training activities. We will seed innovative educational and outreach initiatives that will bring together a wider community including underrepresented groups to enrich their learning and training at the interface of computer and Earth sciences. Specific activities include:

§6.1. DUAL DEGREE CURRICULUM

The computer science department of LSU has already established a dual degree program at graduate level involving computer science and physics. More than 15 students have so far received this degree from the department. The program has been very successful: Its graduates have earned top dissertation honors at the university, and all have got excellent jobs. The PI is currently co-advising one dual-degree student. Given my interdisciplinary interest and research activities, and the existing dual-degree activity of the department; it is a natural strategy to extend the program to encompass the other important discipline of Earth science to which high-performance computing has already contributed substantially.

Proposed Activity: Establish a dual-degree curriculum leading to a Ph.D. in computer science and an M.S. in Earth science: Both the department of computer science, and department of geology and geophysics at LSU are interested in the proposed dual-degree program (see letters from department chairs). Dual-degree students will be exposed to both core and selected advanced courses in computer and Earth sciences. We will:

- Develop a set of interdisciplinary courses, which will form a basis to the dual-degree program: The PI has recently developed/taught a graduate course in scientific visualization (Spring 2003). The course covers visualization principles, techniques, algorithms and tools, which are used to visualize a variety of datasets including multivariate mineral data (e.g., elasticity data). A separate visualization course focused on properties and processes of the Earth and its materials will be developed. The department has already introduced three courses in high-performance computing (I: Fundamental computational techniques required for scientific computing; important algorithms for parallel computation; high performance computing; II: Finite difference schemes for molecular dynamics; classical deterministic simulations; combinatorial optimization; algorithms for quantum molecular dynamics; scientific applications in high performance computing; III: Basic stochastic simulation techniques for massively parallel computers; simulated annealing and routing algorithms). Graduate courses in mineral physics (crystal structure, thermodynamics, elasticity, phase equilibria, rheology), and Earth materials (minerals of crust, mantle and core, and their properties) will be developed in collaboration with Dr. Dutrow (Department of Geology and Geophysics, Louisiana State University).
- Setup the course requirements for the dual-degree program: The above interdisciplinary courses will fulfill partial requirement. A dual-degree student will complete a minimum of 12 semester hours in interdisciplinary courses, which will be counted for both Ph.D. and M.S. requirements. The student will complete a minimum of 9 hours in core courses of geosciences, 6 hours thesis research and 3 hours seminar, thus completing a total of 30 hours for an M.S. in Earth science; whereas he/she will complete the other requirements posed by the department of computer science for the Ph.D. Dr. Dutrow will co-advise M.S. thesis research.
- Supervise two Ph.D. students supported by this career project for the dual-degree program.

- Develop an interactive learning environment for students exploiting the ImmersaDesk facility of LSU. This will involve the development/application of visualization algorithms/software (e.g., Atomic Viewer, Elasticity visualization, Fluid flow visualization) to assist students to explore various phenomena related to the Earth and its materials.
- Involve students in the organization of the proposed workshops, conference and internships (described in the following sections). This will help students develop leadership and communication skills.

§6.2. ACCESS GRID BASED REMOTE TEACHING/LAERNING

An important new concept to fostering education is to offer courses through Access Grid (AG). More recently, the AG is becoming an integral resource of many academic institutions. It is an ensemble of resources consisting of multimedia large-format displays, presentation and interaction environments, and interfaces to Grid middleware and to visualization environments. These resources are used to support group-to-group interactions such as distributed meetings, lectures, seminars, etc. across the Grid. The AG is now used at over 150 institutions worldwide. Each institution has one or more AG nodes, or "designed spaces," that house all the equipments including a large projection wall (18' by 6') and wide seating area (25' by 20'). LSU along with Southern University at Baton Rouge (SU-BR), Southern University at New Orleans (SU-BR) and University of Louisiana at Monroe have recently acquired Access Grid through the support of BRIN (Biological Research Infrastructure Network)-NIH.

The essential idea in an AG-based teaching/learning is that a professor delivers a lecture with students in the AG node at his/her institution and students at other institutions sit in their AG nodes and attend the lecture. The lecturer can use the standard Power Point presentation with any kind of audio and video inputs. The PP slides are projected on the large-format screen in all participating AG nodes in a synchronized manner. The participant students in all AG nodes can lively interact with each other as well as with professor through the Grid. The AG based teaching/learning will thus create an environment for students to take courses, which are not offered by their own institution and also to benefit from seminars delivered by off-campus experts without physically being at the place where the lecture/seminar actually takes place.

Proposed Activity: *Develop an Access-Grid based remote teaching/learning environment at multi-institutional level by including institutions serving underrepresented groups:* This will be an excellent example of integrating information technology into Earth science education, which will provide a unique opportunity to minority students of attending the courses offered through the Grid. We will:

- Initiate Access Grid-based class by offering the scientific visualization course between LSU and SU-BR (see the letter from Dr. Zhao at SU-BR) where at both places the Access Grid node exists. The class will have 20 students including 12 students from LSU and 8 students from SU-BR. The visualization is an ideal course for this kind of initiative as it has a wide range of applications from geophysical, to medical, to financial field, and students from different disciplines will benefit from this course. Moreover, the AG has interface to visualization, which will enable demos of different visualization tools on the Grid.
- Extend this program to include courses at undergraduate level and other institutions (SU-NO, Monroe) in subsequent years. High-performance computing and visualization are areas of broad interest. These courses at graduate and undergraduate level will be offered on the Grid. There will be 40 students in the class counting 10 students from each of LSU, SU-BR, SU-NO and Monroe.
- Provide undergraduate students exciting research experience in Earths materials through the summer internships. This will also help in recruitment of minority students in the proposed dual-degree program. The Louisiana Alliance for Minority Participation (LAMP) summer undergraduate internships supports this type of initiative.



Fig 9. Access Grid at LSU: Consists of a mult display, presentation and interactive environmen lectures, seminars), and interfaces to visuali environments

- Develop a multi-institutional course offering system so that LSU students can benefit from the courses offered by other institutions. This mutual course offering will be helpful in further broadening participation of underrepresented groups.

§6.3. COMPUTATIONAL WORKSHOP FOR UNDERREPRESENTED GROUPS

The PI has co-organized computational science workshop for underrepresented groups that was held, for the second time, at LSU from January 7 to 11, 2003. The workshop brought 22 students and 10 faculty mentors from 12 minority institutions nationwide to Baton Rouge. The number of participations got roughly doubled this time, compared to the first workshop (Fig. 10). This clearly shows the great success of the workshop. Participating students came from varying backgrounds – from freshman to seniors – with majors in computer science, mathematics, geology, physics and biology. The workshop provided students and faculty mentors hands-on training in parallel computing, including construction of a PC cluster. This involved assembling computing nodes from off-the-shelf components, loading the nodes with scientific computing and simulation software, connecting the nodes to fast Ethernet switch, and using this parallel machine for algorithmic and simulation (e.g., molecular dynamics) exercises. It also consisted of a series of lectures on various high-end computational applications on forefronts of materials research. The participants liked the workshop format and are enthusiastic about future activities.



Fig 10. Participants building a PC Cluster in computational science workshop for underrepresented groups

Proposed Activity: Co-organize the computational science workshop for underrepresented groups by further developing the workshop theme: We will

- Add a visualization component to the existing theme of the workshop. This will allow students to visualize live animation of the atomistic (MD) simulations they will be performing. The workshop will also provide hands-on experience with different visualization tools and their applications including those to the Earth materials.
- Give a presentation in the workshop lecture series about rheological properties of Earth materials, which will be carried out under this the proposed project. This will expose the workshop participants to the emerging areas of the computational Earth materials research.
- Setup a special session in the workshop in which LSU researchers and participant minority mentors sit together and discuss on their mutual research interests. It will be a unique opportunity to initiate research collaborations with underrepresented groups.

§6.4 MARDI GRAS CONFERENCE

LSU has established a tradition of bringing together prominent scientists with broad interest and expertise in materials research every year in the name of well-known Mardi Gras Conference for last several years. This international conference was originated and primarily organized in the past by the computational group of Prof. Vashishta, Kalia and Nakano. The PI used to be a senior postdoctoral associate in the group, which has already moved to the University of Southern California (USC) in September 2002. In the process of taking over the conference organizing responsibility, the PI has successfully co-organized the last meeting in February 27 to March 1, 2003. The conference was jointly funded by LSU-CAPITAL and BCVC - the two newly established computational centers with support from the State of Louisiana. The PI has also actively participated in the previous two meetings. The conferences in the past have covered various areas of high-end computational materials research including geophysically relevant materials problems (e.g., mechanical properties). The three-day

conference usually contains about 40 talks (invited and contributed) and about 100 participants including those from LSU.

Proposed Activity: *Continue the Mardi Gras conference and exploit it to bring computational and experimental scientists including those working in mineral physics and Earth science to Baton Rouge from time to time. We will:*

- Co-organize the Mardi Gras conference by closely interacting with the LSU and USC people.
- Add a poster session in which students on- and off-campus will present their research. This will enhance student participation in the conference.
- Enhance participation of SU-BR, SU-NO and Monroe. There were two minority participants in the last meeting from SU-BR.

§7. WORK PLAN

The proposed research and educational activities will be executed following a five-year period work plan outlined in Fig. 11. The QM and MD algorithms will be developed/applied to perform static and dynamics calculations on MgO for benchmarking from the beginning of the project. They will then be applied to MgSiO₃ perovskite. The two techniques will seamlessly be coupled in the second year and the resulting hybrid QM/MD algorithm will be employed to MgO and perovskite in the third and fourth years. Simulations will be carried out on other important mantle minerals including CaSiO₃, SiO₂, wadsleyite and spinel over the last two years.

Year	1	2	3	4	5
Techniques development					
Parallel computing					
QM algorithm	----->				
MD algorithm	----->				
Hybrid QM/MD scheme		----->			
Virtual reality visualization					
Atomistic visualization			----->		
Other techniques					----->
Applications to mantle materials					
MgO				----->	
MgSiO ₃ perovskite				----->	
Other oxides and silicates					----->
Education and outreach					
Dual-degree program					----->
Access-Grid based education				----->	
Computational workshop					----->
Mardi Gras conference					----->

Fig. 11: A 5-year work plan

Visualization of atomistic simulations in immersive and interactive virtual environment will be carried out using and further improving *Atom Viewer* through the first to third year. Different techniques to visualize different scalar, vector and tensor datasets will be developed through the second to fourth year according to the needs imposed by large-scale simulations of minerals.

New interdisciplinary courses will be developed in first and second years. They will be used to implement the proposed dual-degree program from second year. The Access-Grid based teaching/learning system will be initiated in the first year and expanded to the multi-institutional level over the next two years. The computational science workshop for underrepresented groups and Mardi

Gras conference will be held annually. A visualization component will be added to the workshop in the first year and further developed in subsequent years.

REFERENCES CITED

- Allen MP and Tildesley, 1987. *Computer simulations of liquids*, Clarendon, Oxford.
- Bell DR and Rossman GR, 1992. Water in the earth's mantle: the role of nominally anhydrous minerals, *Science*, **255**, 1391-1397.
- Brodholt JP., 1997. Ab initio calculations on point defects in forsterite (Mg_2SiO_4) and implications for diffusion and creep, *Am. Mineral.*, **82**, 1049-1053.
- Brodholt JP, and Refson K, 2000. An ab initio study of hydrogen in forsterite and a possible mechanism for hydrolytic weakening, *J. Geophys. Res.*, **105**, 18,977-18982.
- Chaplot SL and Choudhury, 2001. Molecular dynamics simulations of seismic discontinuities and phase transitions of $MgSiO_3$ from 4 to 6-coordinated silicate via a novel 5-coordinated phase, *Am. Mineral.*, **86**, 752-761.
- Chen G, Liebermann RC and Weidner DJ, Elasticity of single crystal MgO to 8 gigapascals and 1600 kelvins, *Science*, 1998; **280**: 1913-1916
- Dziewonski AM and Anderson DL, 1981. Preliminary reference Earth model, *Phys. Earth Planet. Inter.*, **25**, 297-356
- Eichinger M, Tavan P, Hutter J, and Parinello M, 1999. *J. Chem. Phys.*, **110**, 10452.
- Friedel J, 1964. *Dislocations*, Pergamon.
- Haiber M, Ballone P, and Parrinello, 1997. Structure and dynamics of protonated Mg_2SiO_4 : An ab-initio molecular dynamics study, *Am. Mineral.*, **82**, 913-922.
- Hohenberg P and Kohn W, 1984. Inhomogeneous electron gas, *Phys. Rev. A*, **136**, 864-871
- Ita J and Cohen RE, 1997. *Phys. Rev. Lett.*, **79**, 3198.
- Karato S and Karki BB, 2001. Origin of lateral variation of seismic wave velocities and density in the deep mantle, *J. Geophys. Res.*, **106**, 21771-21783.
- Karato S, Riedel MR, and Yuen DA, 2001. Rheological structure and deformation of subducted slabs in the mantle transition zone: implications for mantle circulation and deep earthquakes, *Phys. Earth and Planet. Int.*, **127**, 83-108.
- Karki BB, 1997. High pressure structure and elasticity of the major silicate and oxide minerals of the Earth's lower mantle, *PhD. Thesis*, University of Edinburgh, Edinburgh, Scotland.
- Karki BB and Stixrude L, 1999. Seismic wave velocities of major silicate and oxide phases of the lower mantle, *J. Geophys. Res.*, **104**, 13025-12033.
- Karki BB, Stixrude L and Crain J, 1997a, Ab initio elasticity of three high-pressure polymorphs of silica, *Geophys. Res. Lett.*, **24**, 3269-3272.
- Karki BB, Stixrude L, Clark SJ, Warren MC, Ackland GJ and Crain J, 1997b. Elastic properties of orthorhombic $MgSiO_3$ perovskite at lower mantle pressures, *Am. Mineral.*, **82**, 635-638.
- Karki BB and Wentzcovitch RM, 2002. First-principles lattice dynamics and thermoelasticity of $MgSiO_3$ ilmenite at high pressure, *J. Geophys. Res.*, **107**, 2267-2273.
- Karki BB and Wentzcovitch RM, 2003. CaO.
- Karki BB, Stixrude L and Wentzcovitch RM, 2001a. Elastic properties of major materials of Earth's mantle from first principles, *Rev. Geophys.*, **39**, 507-534.
- Karki BB, Wentzcovitch RM, de Gironcoli S and Baroni S, 2001b. First principles thermoelasticity of $MgSiO_3$ perovskite: consequences for the inferred properties of the lower mantle, *Geophys. Res. Lett.*, **28**, 2699-2703
- Karki BB, Wentzcovitch RM, de Gironcoli S and Baroni S, 2000. High pressure lattice dynamics and thermoelasticity of MgO, *Phys. Rev. B*, **61**, 8793-8800.
- Karki BB, Wentzcovitch RM, de Gironcoli S and Baroni, S. 1999. First principles determination elastic anisotropy and wave velocities of MgO at lower mantle conditions, *Science*, **286**, 1705-1708.

- Kellogg LH, Hager BH, and van der Hilst RD, 1999. Compositional stratification in the deep mantle, *Science*, **283**, 1881-1884.
- Kohn SC, 1997. Solubility of H₂O in nominally anhydrous mantle minerals using ¹HMAS NMR, *Am. Mineral.*, **81**, 1523-1526.
- Kohn W and Sham LJ, 1965. Self-consistent equations including exchange and correlation effects, *Phys. Rev A*, **140**, 1133-1138
- Manga M, 1996. Mixing of heterogeneities in the mantle – effect of viscosity differences, *Geophys. Res. Lett.*, **23**, 403-406.
- Master G, Laske G, Bolton H, and Dziewonski AM, 2000. The relative behavior of shear velocity, bulk sound speed, and compressional sound velocity in the mantle: Implications for chemical and thermal structure, in *Earth's Deep Interior* (eds. S. Karato et al.), AGU, pp. 63-87.
- Matsui M and Price GD, 1992. Computer simulation of the MgSiO₃ polymorphs, *Phys. Chem. Miner.*, **18**, 365-372.
- Meade C, and Jeanloz R, 1990. The strength of mantle silicates at high pressures and room temperature: implications for the viscosity of the mantle, *Nature*, **348**, 533-535.
- Meade C, Silver PG, and Kershaw S, 1995. Laboratory and seismological observations of lower mantle isotropy, *Geophys. Res. Lett.*, **22**, 1293-1296.
- Merkel S, Wenk HR, Badro J, Montagnac G, Gillet P, Mao HK, and Hemley RJ, 2003. Deformation of (Mg_{0.9},Fe_{0.1})SiO₃ perovskite aggregates up to 32 GPa, *Earth Planet. Sci. Lett.*, **209**, 351-360.
- Merkel S, Wenk HR, Shu J, Shen G, Gillet P, Mao HK, and Hemley RJ, 2002. Deformation of polycrystalline MgO at pressures of the lower mantle, *J. Geophys. Res.*, **107**, 2271.
- Mitrovica JX, and Forte AM, 1997. Radial profile of mantle viscosity: results from the joint inversion of convection and postglacial rebound observables, *J. Geophys. Res.*, **102**, 2751-2769.
- Montagner JP, Where can seismic anisotropy be detected in the Earth mantle? In boundary layers, *Pure Appl. Geophys.*, 1998; 151: 223-256
- Nielsen GM, Hagen H and Mueller H, Scientific Visualization: Overviews, Methodologies, and Techniques, *IEEE Computer Society*, 1997
- Oganov AR, Brodholt JP and Price GD, 2001. Elastic constants of MgSiO₃ perovskite at pressures and temperatures of the Earth's mantle, *Nature*, **411**, 934-937.
- Ogata S, Shimojo F, Kalia RK, Nakano, A, and Vashishta P, 2002. Hybrid quantum mechanical/molecular dynamics simulation on parallel computers: density functional theory on real-space multigrids, *Comp. Phys. Comm.*, **149**, 30-38.
- Poirier JP and Price GD, 1999. Primary slip system of ε-iron and anisotropy of the Earth's inner core, *Phys. Earth Planet. Int.*, **110**, 147-156.
- Payne MC, Teter MP, Allen DC, Arias TA, Joannopoulos JD, 1992. Iterative minimization techniques for ab initio total-energy calculations: Molecular dynamics and conjugate gradients, *Rev. Mod. Phys.*, **64**, 1045-1097.
- Peltier WR, 1998. Postglacial variation in the levels of the sea: implications for climate dynamics and solid-Earth geophysics, *Rev. Geophys.*, **36**, 603-689.
- Schiotz J, Vegge T, De Tolla FD, Jacobsen KW, 1999. Atomic-scale simulations of the mechanical deformations of nanocrystalline metals, *Phys. Rev. B*, **60**, 11971-11983.
- Schroeder W, Martin K, and Lorenzen B, 1997. *Visualization Toolkit: An Object-Oriented Approach to 3D Graphics*, Prentice Hall.
- Sharma A, 2002. Immersive and interactive exploration of billion-atoms systems, *Proc. IEEE Virtual Reality Conference*, Orlando, 217-223.

- Shearer, PM, Upper mantle seismic discontinuities, *In Earth's Deep Interior: Mineral physics and Tomography from the Atomic to Global Scale, Geophys. Monogr. Ser.* edited by S. Karato et al., 2000; 117: 115-131
- Shimojo F, Kalia RK, Nakano A, and Vashishta P, 2001. Linear-scaling density functional-perturbation theory calculations of electronic structure based on real-space grids: design, analysis, and scalability test of parallel algorithms, *Computer Physics Communications*, .
- Sinogeikin SV and Bass JD, Single crystal elasticity of MgO to 20 GPa at high pressure, *Phys. Rev. B*, 1999; 59: 14141-14144
- Stixrude L, and Cohen RE, 1993. Stability of orthorhombic MgSiO₃ perovskite in Earth's lower mantle, *Nature*, **364**, 613-616.
- Svensson M, Hymel S, Froese RDF, Matsubara T, Sieber S and Morokuma, 1996. *J. Comp. Chem.*, **100**, 19357.
- Swygenhoven HV, Spaczer M, Caro A, and Farkas D, 1999. Competing plastic deformation mechanisms in nanophase metals, *Phys. Rev. B*, **60**, 22-25.
- van der Hilst R and Karason H, Compositional heterogeneity in the bottom 1000 kilometers of Earth's mantle: Toward a hybrid convection model, *Science*, 1999; 283: 1885-1888
- Vita AD, Gillan MJ, Lin JS, Payne MC, Stich I, and Clarke LJ, 1992. Defect energetics in MgO treated by first-principles methods, *Phys. Rev. B*, **46**, 12964-12973.
- Wentzcovitch RM, Martins JL and Price GD, 1993. Ab initio molecular dynamics with variable cell shape: Application to study of MgSiO₃ perovskite, *Phys. Rev. Lett.*, **70**, 3947-3950.
- Woo M, Neider J, Davis T and Shreiner D, 1999. *OpenGL Programming Guide: The Official Guide to Learning OpenGL*, Addison-Wesley.
- Yamakov V, Wolf D, Phillpot SR, Mukherjee AK, and Gleiter H, 2002. Dislocation processes in the deformation of nanocrystalline aluminium by molecular-dynamics simulation, *Nature Materials*, **1**, 45-49.