Science and Engineering Visualization Challenge
Entry Form
Entries must be postmarked no later than May 31, 2003
Entries will not be returned

Title of Work: Visualization of Structure-Property Relationships: Spanning the Length Scales (nano to macro)

Entry Category: Photographs ❑   Illustrations   Active and/or Multimedia ❑

Name(s): Ronald D. Kriz_____ Role/title: Associate Professor
Please print

Andrew A. Ray_____ Graduate Student__
Please print

John T. Kelso_____ Senior Research Faculty
Please print

Diana Farkas_____ Professor_____
Please print

Use another sheet for additional team members (see attached).

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I (we) warrant that this entry is original and has been independently developed by me and/or members of my team and does not violate the copyright or other personal or proprietary right of another person or team of people. Further, I (we) attest that I (we) will be able to grant to *Science* and *Science* Online non-exclusive publication and web rights if our entry places first, second or third in any category or honorable mention.

_____   _____

_____   _____

Contact person is responsible for distributing information received from the competition and/or sponsors to all other members of the team.

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Science

Title of Work: Visualization of Structure-Property Relationships: Spanning the length Scales (nano to macro)

Additional Authors

Name(s): Raymond E. Flanery Jr._____   Role/title: Director, Visualization Lab, ORNL
Please print

Descriptive Summary of Submission (100 words): Describe the final product and the basic approach used to create the final product. Also include a succinct description of the resources utilized and a rationale of why the visualization will be an aid to science or engineering and how the concepts are better communicated to the end user.

Recent development of networked collaborative immersive software [1-3] allows more accurate visual analysis of complex connected wave-velocity surfaces propagating through anisotropic crystals. Existing topologies, used for sub-classification within orthorhombic symmetry [4-6], were studied using these immersive tools. From Christoffel's equation the fourth order elastic stiffness tensor, C_{ijkl}, uniquely defines these topologies where the collection of all wave speeds, v, (topology) and their vibration directions, α_k, correspond to the wave propagation direction, ν_k, and color is defined by $\alpha_k \nu_k$ [7]. Together both topology and color uniquely represent C_{ijkl} for Ca[HCOO]2. Insight occurs when the observer is "immersed" inside the crystal (nano-structure) and the wave velocity (macro-property) topology. Polar covalent bond orientations are seen to align along stiffer directions where faster longitudinal wave speeds appear as purple bulges.

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5. Ledbetter, H.M. and Kriz, R.D, "Elastic-Wave Surfaces in Solids", *Physica Status Solidi*, Vol. 114, pp. 475-480, 1982.

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7. Kriz, R.D., Farkas, D., Batra, R.C., "NSF - Combined Research and Curriculum Development: Computer Simulation of Material Behavior - From Atomistic to the Continuum Level", course module: Introduction to Mechanical Behavior of Anisotropic Materials (2002): http://www.jwave.vt.edu/crcd/kriz/lectures/Anisotropy.html

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- If an insufficient number of qualified entries are received, the sponsoring organizations reserve the right to modify or cancel the competition prior to announcing winners.
- Expenses paid by the National Science Foundation for travel to Washington, D.C., will be within the limits set forth in law according to the Federal Travel Regulations.
- All contestants agree that they, their heirs, and estates shall hold harmless the United States, the employees of the federal government, and all employees of the National Science Foundation, *Science* and *Science* Online for any and all injuries and/or claims arising from participation in this contest, to included that which may occur while traveling to or participating in contest activities.
- The National Science Foundation will fund travel for only one person per group or team entry if the entry wins. This person will be the contact person listed on the entry form. If this person is not available, he/she will designate a replacement from the team. If a single person wins multiple categories, he/she must represent all of the winning entries; designees are not permitted in this instance. Only persons listed on the original entry form may have their travel funded by the National Science Foundation. All other persons accompanying winner/group representative must arrange and fund their own travel and accommodations.