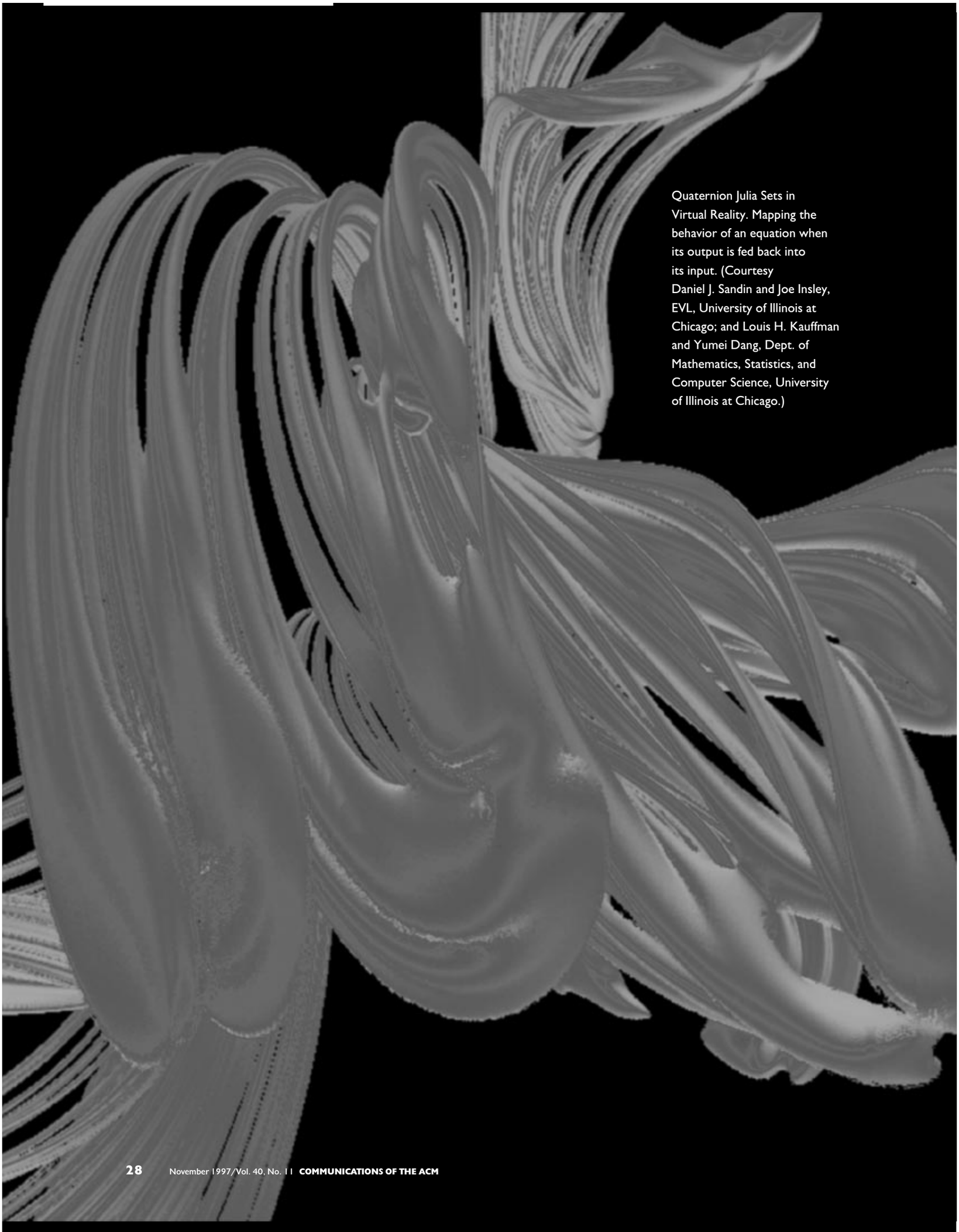
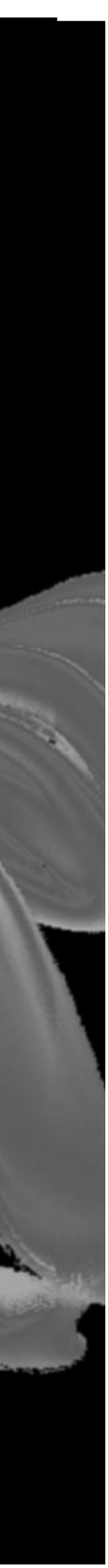


Quaternion Julia Sets in Virtual Reality. Mapping the behavior of an equation when its output is fed back into its input. (Courtesy Daniel J. Sandin and Joe Insley, EVL, University of Illinois at Chicago; and Louis H. Kauffman and Yumei Dang, Dept. of Mathematics, Statistics, and Computer Science, University of Illinois at Chicago.)

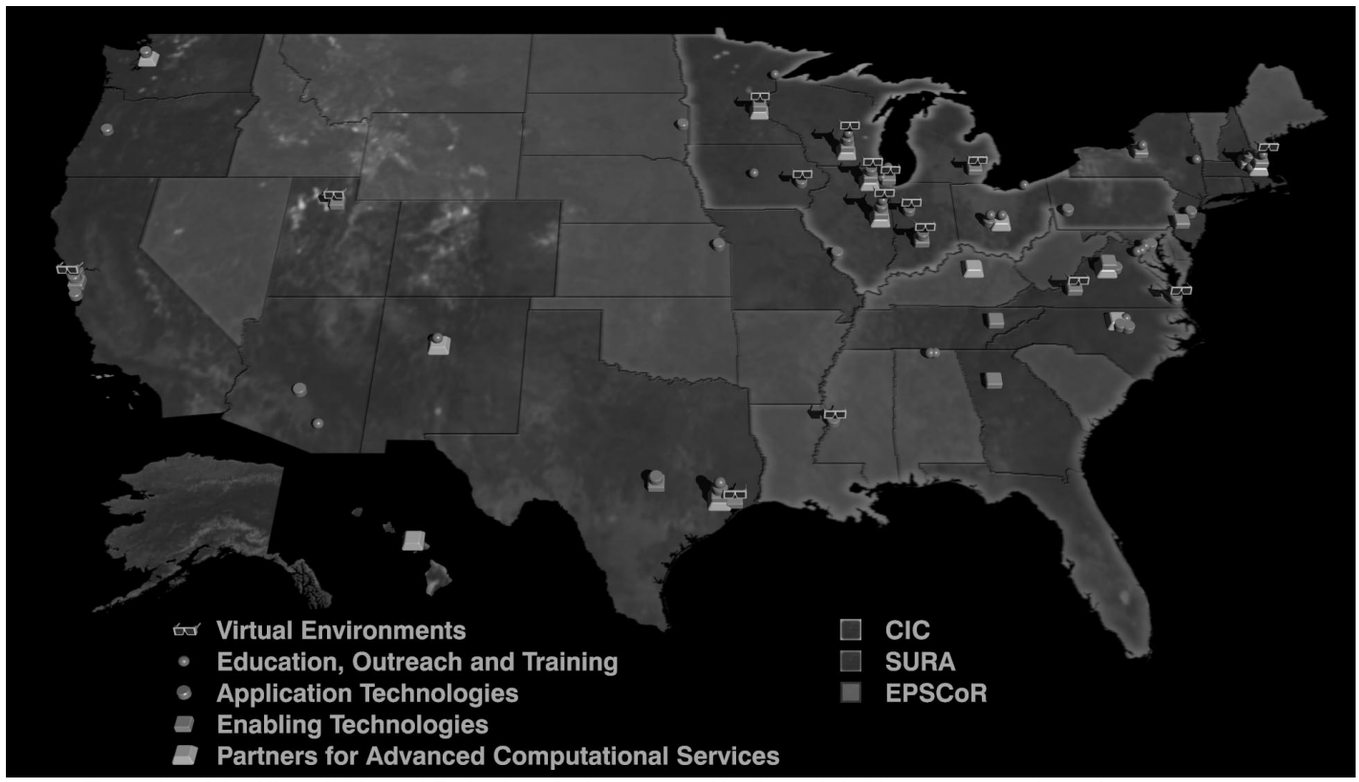


Computational Infrastructure

Toward the 21st Century

During the past 10 years, the U.S.'s computational infrastructure has been transformed from isolated computational centers of excellence to a fully distributed web of computer-mediated knowledge. The National Science Foundation Supercomputing Centers have been at the forefront of this transformation by constructing the first NSFnet backbone network, turning printouts into scientific visualizations, and developing new community software—from Telnet in the 1980s to Mosaic in the 1990s. In 1985, when the NSF Supercomputer Centers were opened, cyberspace was a wasteland; by 1995 it had become an urban sprawl. Frontier Centers were appropriate in 1985; virtual distributed partnerships were the correct format 10 years later.

Larry Smarr, Guest Editor



COURTESY ROBERT PATTERSON, NCSA

The nodes of the Alliance's National Technology Grid consisting of hardware (a highly interconnected set of supercomputers, virtual environments, and massive datastores) and of people (the Alliance partners described in the articles in this section)

The National Computational Science Alliance, one of the new NSF Partnerships for Advanced Computational Infrastructure (PACI), now has a detailed plan for creating a National Technology Grid to provide desktop access to the most powerful computational science and engineering problem-solving environment ever assembled. The Alliance will strive to make computing routinely parallel, distributed, collaborative, and immersive. The plan's key feature is that the new infrastructure is application-driven through close coupling to the needs of the user community. The Grid, like the earlier Supercomputer Centers program will be open to the national research community for innovative computer science experiments and enable remote users to attack heretofore intractable science and engineering problems (see Figure).

The two winning proposals for the PACI program began operation October 1, 1997. I direct the Alliance, with its leading-edge center at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign (see http://Aliance.ncsa.uiuc.edu). The other one, directed by Sid Karin, a professor of computer science and engineering at the University of California at San Diego, is called the National Partnership for Advanced Computational Infrastructure (NPACI), managed by the University of California at San Diego with its leading-edge center at the University's San Diego Supercomputer Center (see http://www.npacia.edu). Over the next five years, NSF will provide approximately $170 million for each, or a total not to exceed $340 million.

Why the Grid?

The Alliance includes a broad range of individuals and institutions brought together to create a new intermediate step between basic research and vendor-produced products. The Grid is a persistent evolving prototype of the early 21st century computational and information infrastructure. The goal is to make this national-scale metacomputer as usable as standalone supercomputers were during the past decade. Achieving such a multi-year evolution of the U.S. computational fabric requires an infrastructure of people (the Alliance) and technology (the Grid) that will do a great deal to maintain the U.S.'s position as the global leader in computational science and engineering research.

The Grid, prototyped by the Alliance, along with similar efforts by NPACI, will serve as an early

model for a full-scale advanced computational infrastructure, which will be built jointly by computer, communications, and software vendors to support U.S. computational scientists and engineers in universities, industry, and government. The national-scale Grid emerges from the Alliance's Leading Edge facilities and its Advanced Hardware partners, including a broad range of the most powerful high-performance architectures—the Grid's Supernodes—that will be accessed by thousands of remote computational science and engineering users. Using such high-performance networks as the NSF's vBNS, the Grid will link the Supernodes to dozens of visualization and virtual reality displays, massive data stores, and remote instruments. Alliance-developed, object-oriented software "glue" will unify these resources for collaborative problem-solving, from the desktop to tele-immersion.

The Alliance is anchored at NCSA and is composed of researchers at more than 50 university, national laboratory, and Industrial Partner sites. It also includes educational leaders, state and regional centers, and associations of universities and of states. Grid software development will be carried out by dozens of leading researchers in computer science (Enabling Technologies, or ET, teams), computational science and engineering (Application Technologies, or AT, teams), and computer, communications, and software industries (Strategic Vendor partners) to jointly produce a national-scale plan for implementing the Grid.

This special section of *Communications* is devoted to exploring in some detail Alliance plans for the next five years. The ET team leaders are the authors of three articles, revealing how they will design and deploy the Grid infrastructure (led by Rick Stevens of Argonne National Laboratory); integrate data management, virtual environments, and collaborative technologies within the Grid (led by Dan Reed of the University of Illinois at Urbana-Champaign); and bring software scalability to the shared memory computers of the Grid's Supernodes (led by Ken Kennedy of Rice University).

These three computer science teams are working with leading application researchers organized into the six AT teams—Cosmology, Environmental Hydrology, Chemical Engineering, Molecular Biology, Nanomaterials, and Scientific Instrumentation. These areas were carefully chosen to span disciplines and infrastructure needs while building on Alliance strengths. They are introduced by Greg McRae of MIT in an article looking closely at his Chemical Engineering team; the Cosmology Team's plans are detailed by Jeremiah Ostriker of Princeton University and Michael Norman of NCSA. As early users of the emerging Grid, the AT teams will challenge existing paradigms, driving the ET teams' development of innovative software, database tools, novel algorithms, and collaborative problem-solving environments. As with the ET teams, funding for their underlying basic scientific research will be provided by the researchers themselves from other funding sources following the traditional peer-review process.

The Alliance will strive to make computing routinely parallel, distributed, collaborative, and immersive.

Positioning for the 21st Century

Because today's high-performance technologies give us an early look at tomorrow's mass-market capabilities, the Alliance will partner with many sectors of society to accelerate adoption of these new technologies. NCSA's 10-year Industrial Partner and Strategic Vendor programs ensure early involvement by the corporate sector in Grid design and development.

The Alliance is nationally distributed and broadly based. Participation of experienced leaders in grade school, undergraduate, and graduate education; federal, state, and local governments; and

It needs to be understood up front that this is a radical and visionary plan for the U.S. never tried before on a national scale across so many disciplines.

businesses of all sizes will provide organized active content to the Grid reflecting the regional, cultural, and intellectual diversity that is the U.S.'s national strength. The Grid links Alliance components while providing access to its resources to the national user community. We will design the Alliance and the Grid in a manner that is accessible to all. Moreover, the Alliance is committed to increasing participation of groups (particularly women and minorities) and institutions historically underrepresented in advanced computation.

Recognizing that it takes a virtual organization to build a virtual machine, the primary responsibility for overall Alliance management and planning lies with its Director, the Deputy Directors, and the Alliance Executive Committee, which consists of 14 members from the academic and industrial computational and computer science and engineering communities with extensive experience in managing large research projects and high-performance computing centers. The co-authors of the articles in this issue are either members of the ETs or NCSA senior staff responsible for implementing Alliance plans. Oversight is provided by the Alliance's External Advisory Council, whose chair Philip Smith offers a short article placing the PACI program in its historical context.

It is important to remember that what is presented in these articles is a proposed program of infrastructure development by a virtual national team. They are inspired by the notion of continually harvesting the advances made by peer-reviewed basic research and its integration into the Grid so the new capability can be accessed, exploited, and judged by a wide range of users as part of an integrated whole. It needs to be understood up front that this is a radical and visionary plan for the U.S. never tried before on a national scale across so many disciplines. We will make mistakes along the way, but what we learn from these mistakes and from our successes will greatly empower the research community as well as U.S. industrial competitiveness.

We are convinced by our accumulated experience that both hardware and software can be advanced most efficiently by users striving to solve complex, cutting-edge computational problems. Therefore, our plan can be realized only through an Alliance of researchers with experience shaping both computational science and computer science. Even more important, Alliance members have been chosen because of their personal commitments to working together, enabling dramatic advances by a new level of national-scale multidisciplinary collaborative research.

The vision for the Alliance is to enable the science and engineering community to reap the benefits of rapidly improving high-performance computing and communication technologies by prototyping the computational and information infrastructure needed for the 21st century and rapidly transferring these developments to the broader society. C

Larry Smarr (pls@ncsa.uiuc.edu) is Director of the NCSA at the University of Illinois at Urbana-Champaign and was recently appointed to the Presidential Advisory Committee on High-Performance Computing and Communications, Information Technology, and the Next Generation Internet. His most recent book (with William Kaufmann III) is *Supercomputing and the Transformation of Science*.

The NSF PACI award for NCSA's proposed "National Computational Science Alliance" became effective October 1, 1997. NCSA receives major funding from the NSF, DARPA, NASA, Defense Dept.'s Modernization Program, other federal agencies, corporate partners, the University of Illinois, and the State of Illinois.