First Steps for the Rational Design of Drugs
In a pioneering effort that allowed scientists to visualize the behavior of key biological molecules in the body, a team of scientists—using supercomputing resources at SDSC—took an important first step in the relatively new arena of rational drug design. In a paper published in the journal Science, the team—which included Paul Bash, Peter Kollman and Robert Langridge of UCSF and U. Chandra Singh with the Scripps Clinic—reported that they had determined the relative free energies of binding for different chemical inhibitors at the same active molecular site. The result was significant since what makes one drug more powerful or effective than another is that, at the molecular level, it binds more readily at the site at which it acts.

Engineering Designer Plants
It’s the most abundant protein found in nature, with a whimsical name reminiscent of the company best known for its cookies. But more important than its mere abundance, RuBisCO is the key enzyme in the initiation of photosynthesis, the process by which green plants make usable energy from sunlight. In 1988, with the help of a new detector for x-ray crystallography and SDSC’s CRAY X-MP, a team of scientists led by Chapman et. al. reported, for the first time, the three-dimensional structure of RuBisCO, with a subsequent goal of building a new, improved RuBisCO to engineer designer plants that would photosynthesize more efficiently, creating more food for a hungry world.

Atmospheric Carbon Dioxide from Fossil Fuels
Beginning in the late 1950s, Charles Keeling from UC San Diego’s Scripps Institution of Oceanography (SIO) continuously collected data on the distribution of carbon dioxide around the globe. In 1989, Keeling—with SIO colleagues Stephen Piper and Robert Barcastos, using SDSC resources—constructed a three-dimensional computer model of the terrestrial carbon cycle that took advantage of the data collected by Keeling. The model was the first to confirm the importance of fossil fuel combustion in loading the atmosphere with carbon dioxide, especially over the northern hemisphere.
1988

UCSD/SDSC Researchers Solve Structure for the Body’s “Transistors”
Protein kinases have been likened to cellular regulatory circuits in living organisms that perform similar functions as transistors or chips in a computer. In 1991, a team of researchers from SDSC and UCSD reported in a cover story in *Science* that they had solved its three-dimensional structure; the solution—with the aid of the CRAY supercomputer at SDSC and a stereoscopic visualization system in SDSC’s Advanced Scientific Visualization Lab (VizLab)—was considered one of the Grand Challenges of computational and biological science.

Researchers around the globe then began searching for specific kinase inhibitors that target specific diseases, including diabetes and tumor initiation and growth.

1991

CERFnet officially dedicated at SDSC: Vinton Cerf (no relation to the network) conducts dedication.

CRAY Y-MP8/864 supercomputer arrives at SDSC and made available December 22.

3-D structure of RuBisCo, the key enzyme in the initiation of photosynthesis and most abundant protein found in nature, is solved with aid of SDSC supercomputers and published in *Science*.

Charles Keeling, et. al., with SDSC supercomputers, construct 3-D model of the terrestrial carbon cycle confirming the importance of fossil fuel combustion in loading the atmosphere with carbon dioxide.

Dave Nadeau and Holliday Horton at SDSC create an animation of accretion disks – the fiery nebulae and spinning clouds in a primordial solar system – for a planetarium show at S.D.’s Reuben H. Fleet Space Center and Theatre.

NSFnet backbone becomes a production network.

KidLab, an after-school program for 10-12 year olds, established at SDSC.

1992

SDSC Takes Big “STEP” with Innovative Program for Local Teachers
With the beginning of the 1992 school year, SDSC launched its Supercomputer Teacher Enhancement Program (STEP) and presented its first half-day-in-service to 25 educators and parents from Grant Math Science Magnet School. The program—a forerunner to SDSC’s award-winning TeacherTech program—was designed to show teachers how scientists use computers to make discoveries, and it introduced teachers to ways elementary school students could use computers to learn about math and science.

SDSC acquires 32-node iPSC/860 parallel computer from DARPA, built by Intel.

SDSC acquires 256-node NCUBE 2 parallel computer.

1995

Catching an Alleged Cyber-criminal
On February 15, 1995, SDSC Senior Fellow Tsutomu Shimomura and Systems Analyst Andrew Gross collaborated with federal agents to track down alleged computer criminal Kevin Mitnick. Shimomura and Gross applied their knowledge of computer network security to help agents apprehend Mitnick, then considered the “most-wanted computer criminal in the United States,” after an intruder broke into a network of computer systems at Shimomura’s home and at SDSC. Mitnick, now a computer consultant and author, was convicted of various computer- and communications-related crimes; he was released from prison in January 2002.
Catching a Speeding Enzyme in the Act

With large-scale computer simulations run at SDSC, researchers showed how one of the fastest enzymes–acetylcholinesterase (AChE), which controls communications among nerves and muscle cells–works. The speed of AChE had been puzzling, since its active site appeared to be accessible only by a partly blocked channel on the enzyme’s surface. Earlier work showed that “breathing” motions in AChE open and close the channel to allow acetylcholine (ACh) to enter the active site. The new work showed that the breathing motions allowed ACh to bind almost as fast as if the channel were always open. A team of researchers, including J. Andrew McCammon (UC San Diego) combined computational models and theoretical calculations to obtain their results, published in the August 4 Proceedings of the National Academy of Sciences.

SDC Releases Glue that Holds Data Together

In 1998, the Storage Research Broker (SRB) 1.1 was released as the “middleware” that holds together data cache sites for NPACI, the National Partnership for Advanced Computational Infrastructure. The SRB software, built on the work of Reagan Moore at SDSC, is still used by many U.S. and international computational science research projects. It is considered a “middleware” in the sense that it is built on top of other major software packages (various storage systems, real-time data sources, etc.) and it has callable library functions that can be used by higher-level software. SDSC’s Chaitan Baru, Michael Wan, Arcot Rajakser and Wayne Schroeder were members of the original team that developed SRB.

Computer Simulations Reveal New Anti-HIV Strategy, Leading to AIDS Drug

Molecular dynamics simulations, conducted by a team led by UCSD chemist J. Andrew McCammon, provided new insights into attacking a third target against HIV—integrase—that helps the virus hijack the body’s cells. The simulations, published in 1999 in the Biophysical Journal, led to the development of Isentress, marketed by Merck as a new HIV drug approved for patient use by the FDA. Hailed as the most important new AIDS drug in a decade, the drug was the first AIDS medicine to block integrase, considered crucial in the process HIV uses to replicate.
1994

A data transfer speed record of 630 Mb/s is achieved across the 100-mile CASA Gigabit Testbed link between SDSC and Caltech, accelerating solution of the reaction of atomic hydrogen with molecular heavy hydrogen (deuterium) by a factor of 3.3.

1995

The cover of Chemical and Engineering News features an image of cyclohexatriene molecule; research results from computational and experimental collaboration of Kim Baldridge at SDSC and Jay Siegel, at UCSD.

1996

SDSC receives $8.4M contract from DARPA to develop Distributed Object Computation Testbed (DOCT) for handling complex documents on geographically distributed data archives and computing platforms; to focus on the needs of the US Patent and Trademark Office.

1999

World's Largest Repository of Protein Structures Housed at UCSD/SDSC

On July 1, 1999 responsibility for the Protein Data Bank (PDB)—the world's largest archive for biomedical structures—formally shifted to the Research Collaboratory for Structural Bioinformatics (RCSB) with a new PDB website and ftp archive. Today, the program is managed jointly by two partner sites: Rutgers University, under the direction of Helen Berman; and SDSC and the Skaggs School of Pharmacy and Pharmaceutical Sciences at UCSD. The PDB houses about 100,000 biological structures, including proteins associated with the common cold, avian flu, HIV, West Nile virus, Alzheimer's disease, and a wide variety of cancers.

Chris Mihos and Lars Henquist of UC Santa Cruz collaborate with computer artists at NCSA, using computational resources at SDSC CRAY C90, to create high-resolution images of a galaxy encounter for IMAX cosmic voyage, which debuts at the Smithsonian National Air and Space Museum in D.C.

SDSC establishes the telemanufacturing facility to rapidly prototype 3D models from digital geometry data.

For the first time, SDSC harnesses the power of a new very high-speed network (vBNS) by distributing portions of a computation across high-performance computers located on the east and west coasts.

Tsutomu Shimomura, SDSC Senior Fellow, collaborates with federal agents to track down alleged “notorious cybercriminal” Kevin Mitnick, then considered the “most-wanted computer criminal in the United States.”

A model of the nicotinic acetylcholine receptor is developed by Igor Tsigelny, Naoya Sugiyama and Palmer Taylor at UCSD/SDSC, in collaboration with Steven Sine at the Mayo Foundation; enzyme is a target for addictive activity from nicotine.

2000

Transporting Theater-goers at Hayden Planetarium to the Orion Nebula

Astronomically accurate visualizations made possible for the first time by SDSC researchers and the IBM Blue Horizon supercomputer at SDSC transported space theater visitors to the Orion Nebula—the first destination of the virtual starship departing from the reopened Hayden Planetarium at the American Museum of Natural History in New York. The visualizations were made possible by SDSC's Galactic MPIRE volume-rendering software package, under the technical leadership of SDSC's Dave Nadeau.

SDSC Technologies Provide Huge Image Archive to Study Human Embryology

SDSC-developed storage and visualization technologies were integrated into a National Library of Medicine project to create one of the largest-ever medical image databases. The project, called “Human Embryology Digital Library and Collaboratory Support Tools,” was designed to demonstrate how leading-edge information technologies in computation, visualization, collaboration, and networking can expand the capabilities of medical science in developmental studies, clinical work, and teaching. The database allowed project participants to study data sets of sizes up to a terabyte, in multi-gigabyte images, using the IBM HPSS archival storage system at SDSC, the Storage Resource Broker, and the MPIRE 3-D system to support the 3-D rendering of data.

NIH approves $3.286M to SDSC to fund the National Biomedical Computation Resource (NBCR).

Thinking Machines CM-2 arrives at SDSC to support UCSD education and research.
Under the leadership of Phillip Papadopoulos at SDSC, the National Partnership for Advanced Computational Infrastructure (NPACI) designed and released an enhanced version of the NPACI Rocks Cluster Toolkit, a set of open-source enhancements for managing Linux-based computer clusters. Over time, Rocks—simple, self-contained, scalable and upgradable—slowly became the de facto software package for implementing clusters. By the end of 2001, NPACI Rocks was used to establish clusters at the Pacific Northwest National Laboratory, Northwestern University, the University of Texas, and Caltech.
In the Beginning...
Michael Norman, professor of physics at the Center for Astrophysics and Space Sciences (CASS) at UC San Diego, together with colleagues at CASS and SDSC, ran the world's largest and most complex scientific simulation of the evolution of the universe ever performed. Using SDSC's IBM Blue Horizon supercomputer, the team tracked the formation of enormous structures of galaxies and gas clouds during the millions and billions of years following the Big Bang. Norman ran his "Enzo" cosmology program for more than 100 hours on all 128 computing nodes of the Blue Horizon.

Envisioning the “Big One” for Southern California
A collaboration of 33 earthquake scientists, computer scientists, and others from eight institutions produced the largest and most detailed simulation yet of just what might happen during a major earthquake—magnitude 7.7—on the southern San Andreas Fault. The simulation, known as TeraShake, used the new 10 teraflops IBM DataStar supercomputer and large-scale data resources of SDSC. The simulation provided more detail into how intensely the earth would shake during such an event, and what impact it would have on structures, particularly in the populated sediment-filled basins of Southern California and northern Mexico.

Predicting “Solar Storms”
At times, “solar storms” ejected from the sun’s corona—it’s ghostly outer atmosphere—can eject plasma in the direction of the Earth, resulting in potentially serious disruptions in satellite operations, communications, and even electrical power grids. Since society is heavily dependent on these infrastructures, predicting "solar storms" are of tremendous importance. The March 29, 2006 solar eclipse gave scientists from the Solar Physics Group at SAIC (Science Applications International Corporation) an opportunity to check their predictions of the state of the solar corona based on a computational model using observed photospheric magnetic field data. Using dedicated time on SDSC’s IBM supercomputer DataStar and NASA’s Columbia system, this work represented the most true-to-life computer simulation ever made of the solar corona.
Predicting Protein Structure in Record Times

Researchers from SDSC, contributing their massive computational capabilities to a collaboration with colleagues at the University of Washington and IBM, helped achieve the largest-ever protein structure prediction—and completed the complex simulation in less than three hours, a task that previously took weeks. The ground-breaking demonstration used UW Professor David Baker's Rosetta Code and ran on more than 40,000 central processing units of IBM’s Blue Gene Watson supercomputer, using the experience gained on the IBM’s Blue Gene system at SDSC. Ross Walker, a SAC computational scientist at SDSC, managed the Baker’s group access to SDSC machines, helping them to optimize their code.

HPWREN Comes to the Aid of Local Fire Fighters

Firefighters facing fast-spreading wildfires, especially in remote areas where communications and other resources are scarce, added “cyberinfrastructure” to their firefighting arsenals during the 2006 “Horse Fire” in California’s Cleveland National Forest. Experts from the High Performance Wireless Research Educational Network (HPWREN)—a resource supported by the NSF and staffed by researchers at SDSC, Scripps Institution of Oceanography, and San Diego State—responded to the urgent request of state firefighters for quick and reliable wireless communications among widespread teams. Within a day, HPWREN experts were on the scene, establishing high-speed wireless data links needed to contain the flames.

Zeroing in on the Cause of Alzheimer’s and Parkinson’s Disease

Scientists led by UCSD’s J. Andrew McCammon use molecular simulations and SDSC resources to identify a potential mechanism underlying the drug resistance of the worst mutant HIV strain; in same work, the researchers identify a separate region of protease enzyme that might serve as new drug target.

SDSC launches DataCentral, the first program of its kind to support large community data collections and databases.

Data experts at SDSC collaborate with American Red Cross to help locate missing loved ones in the wake of Hurricane Katrina; results in “Safe and Well” website.

CENIC announces that the first production 10 Gigabit Ethernet campus connection in the U.S. has been installed from UCSD.
Setting Records for “Virtual Weather” Prediction

A team of researchers from SDSC, the National Center for Atmospheric Research (NCAR), Lawrence Livermore National Laboratory, and the IBM Watson Research Center set U.S. records for size, performance, and fidelity of computer weather simulations, modeling the kind of “virtual weather” that society depends on for accurate weather forecasts. The research, led by Allan Snavely at SDSC, was a finalist for the Gordon Bell Prize.

Removing Bottlenecks from the Internet

SDSC/CAIDA researchers Dmitri Krioukov and Kimberly Claffy, along with Marián Boguñá (Universitat de Barcelona), reveal in Nature Physics a previously unknown mathematical model called “hidden metric space” that may explain the “small world phenomenon” that society depends on for accurate weather forecasts; a finalist for Gordon Bell Prize.

Modeling Earth’s Enigmatic Core

To learn more about the inner sanctum of the earth’s core, seismologists take advantage of one of nature’s most destructive forces: earthquakes. Somewhat like the way a CAT scan images the brain, seismologists track seismic wave patterns from earthquakes to model the structure of the earth’s core. One of the great challenges is to capture the propagation of high-frequency waves, with periods of 1 to 2 seconds, as they travel across the globe. In 2008, a team of researchers from SDSC employed a spectral-element application called SPECFEM3D_GLOBE to complete record-setting, petascale-level simulation of the earth’s inner structure; a finalist for Gordon Bell Prize.
SDSC unveils Dash, a “flash-memory-based” supercomputer to accelerate solutions for data-intensive science problems.

The CIPRES portal, used to help researchers track evolutionary relations among species, becomes the most heavily used portal in the TeraGrid, accounting for 20% of active TeraGrid users during the first quarter of 2010.

Researchers at SDSC, SDSU and UCSD create the largest-ever simulation of a Magnitude 8 earthquake, primarily along the southern section of the San Andreas fault.

Researchers from UC Irvine, led by Rommie Amaro and using SDSC expertise and resources, find a new approach to create customized therapies for virulent flu strains that resist current antiviral drugs. The findings were published in Nature Communications.

The Center for Large-scale Data Systems Research (CLDS), bringing together industry and university research to investigate “big data” challenges, is launched under the direction of SDSC researcher Chaitan Baru.

Mike Norman named SDSC director.

SDSC completed a comprehensive upgrade to its tape-based archival storage capacity, increasing its total to 36 petabytes, the largest digital storage capacity of any academic center in the world.

SDSC officially launches the Triton Resource, an integrated data-intensive computing system primarily designed to support UCSD and UC.

2009

Providing a Portal to Build the Tree of Life

To help scientists build the Tree of Life—to infer the evolutionary history of Earth’s myriad species starting from biomolecular sequence data—the NSF funded a project called CIPRES (CyberInfrastructure for Phylogenetic RESearch). As part of this project, SDSC developed the CIPRES portal—a browser interface to the most widely used phylogenetic codes—along with faster versions of these codes. In December 2009 the portal was migrated to the TeraGrid, the nation’s largest open-access network of high-performance computers. Within the first quarter of 2010, the portal had 500 users, the most of any TeraGrid portal and 20 percent of all active TeraGrid users. Each month since then, more than 100 new users have accessed TeraGrid resources through the portal, attesting to the broad impact of this enabling interface.

2010

Using Simulations to Create Customized Therapies for Virulent Flu Strains

The search for effective flu drugs has always been hampered by the influenza virus itself, which mutates from strain to strain, making it difficult to target with a specific pharmaceutical approach. Researchers from UC Irvine, with assistance of SDSC expertise and computer resources, found a new approach to create customized therapies for virulent flu strains that resist current antiviral drugs. The findings, published in Nature Communications, offered an avenue to build new drugs that exploit so-called flu protein ‘pockets.’ Using powerful computer simulations on SDSC’s Trestles system, UC’s Rommie Amaro and Robin Bush with SDSC’s Ross Walker created a method to predict how pocket structures on the surface of influenza proteins promoting viral replication could be identified as these proteins evolve, allowing for possible pharmaceutical exploitation.

2011

Internet Censorship Revealed Through a Maze of Malware

In January 2011, Egypt—with 23 million Internet users—vanished from cyberspace after its government ordered an Internet blackout amidst anti-government protests. The following month, the Libyan government, also under siege, imposed an Internet “curfew” before completely cutting access for almost four days. To help explain how these governments disrupted the Internet, a team of scientists led by kc Claffy, director and founder of CAIDA at SDSC, conducted an analysis based largely on the drop in a specific subset of observable Internet traffic that is a residual product of malware. Their analysis, funded by the NSF and Department of Homeland Security—and including scientists from Italy and The Netherlands—was the first published research to demonstrate how malware-generated traffic pollution could be used to analyze Internet censorship and other macroscopic network outages.
A study led by SDSC’s James Short predicts that by 2015, the sum of media delivered to consumers on mobile devices and to their homes would take 15+ hours a day to consume. That’s equal to nine DVDs worth of data per person per day.

The NSF awards SDSC a $12 million grant to deploy Comet, a new petascale supercomputer designed to transform advanced scientific computing by expanding access and capacity among traditional as well as non-traditional research domains.

Researchers from SDSC, the U.S. Geological Survey, and the San Diego Zoo’s Institute for Conservation Research develop methodology that for the first time combines 3D and advanced range estimator technologies, providing detailed data on the movements of terrestrial, aquatic, and avian wildlife species.

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A published global genome study using SDSC’s data-intensive Gordon supercomputer have researchers rethinking how avian lineages diverged after the extinction of the dinosaurs. The four-year project, called Avian Genome Consortium, is published in the journal Science in late 2014.

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WIFIRE, designed to build a cyberinfrastructure to perform real-time data-driven assessments of wildfires, is funded under a three-year NSF grant to SDSC, Calit2/Qualcomm Institute, and the Jacobs School of Engineering’s MAE department. Also participating is the University of Maryland’s Department of Fire Protection Engineering.

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About this Brochure

On November 14, 1985, the San Diego Supercomputer Center opened its doors on the northwestern corner of the UC San Diego campus and showed off its first supercomputer, a CRAY X-MP/48 — clocking at what one newspaper article called a “mind-boggling” billion calculations per second... a gigaflop. Actually, the peak performance was closer to 800 million calculations per second, but still pretty fast then. Some 100 researchers — all from traditional disciplines such as astrophysics, biochemistry, geology, and oceanography — applied for time on the new supercomputer, which promised to usher in a new era of scientific discovery.

Since that day, scientific and technological advances made possible, and/or created by SDSC staff and resources like the original CRAY, have made a major mark in academia, industry, and society-at-large — “turning data to discovery,” a phrase that has become associated with SDSC. The Center has brought together researchers at UC San Diego and across the nation and world, in partnerships and collaborations that now are the hallmark of today’s scientific enterprise. SDSC also has proven to be a good neighbor, providing its expertise and considerable resources to local educators and students, firefighters and other “first-responders,” families of military serving overseas, and others in time of need.

To help commemorate SDSC’s 30th anniversary, SDSC has pulled together a timeline of the most significant events in the Center’s history. This timeline, now located outside SDSC’s data center in the building’s East Wing addition, serves as a physical reminder of the historical milestones that have made SDSC a local, state, and national resource for high-performance and data-intensive computing, and a leader in research and development of the nation’s vast cyberinfrastructure.

As an added element to this celebration, this brochure spotlights 30 significant moments and/or advances in science, technology, and outreach made possible by the Center and its staff. The “Top 30” list, published in this document, represents but a small sampling of the hundreds of major accomplishments over SDSC’s history; clearly, many other achievements also deserve recognition. We are confident this list will be discussed and debated, and ultimately revised and updated when the next such list is developed!

SDSC
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