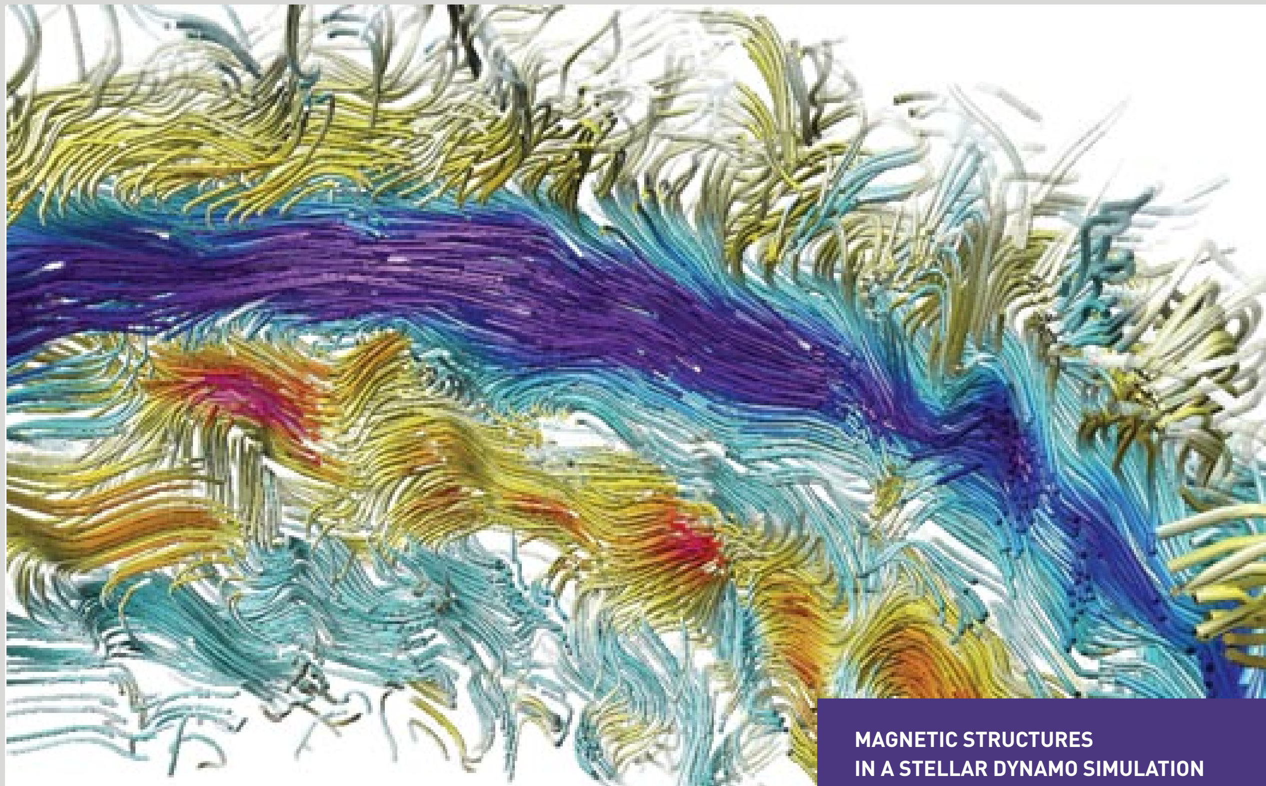
SOLAR DYNAMO



MAGNETIC STRUCTURES IN A STELLAR DYNAMO SIMULATION

Stars generate magnetic fields through turbulent convection in their interiors that, as if pulling taffy, stretches, twists, and amplifies magnetic flux. This image shows magnetic lines of force in the convection zone of a rapidly rotating star, with colors (red positive, blue negative, white neutral) indicating direction. (Created by Ben Brown using VAPOR.)

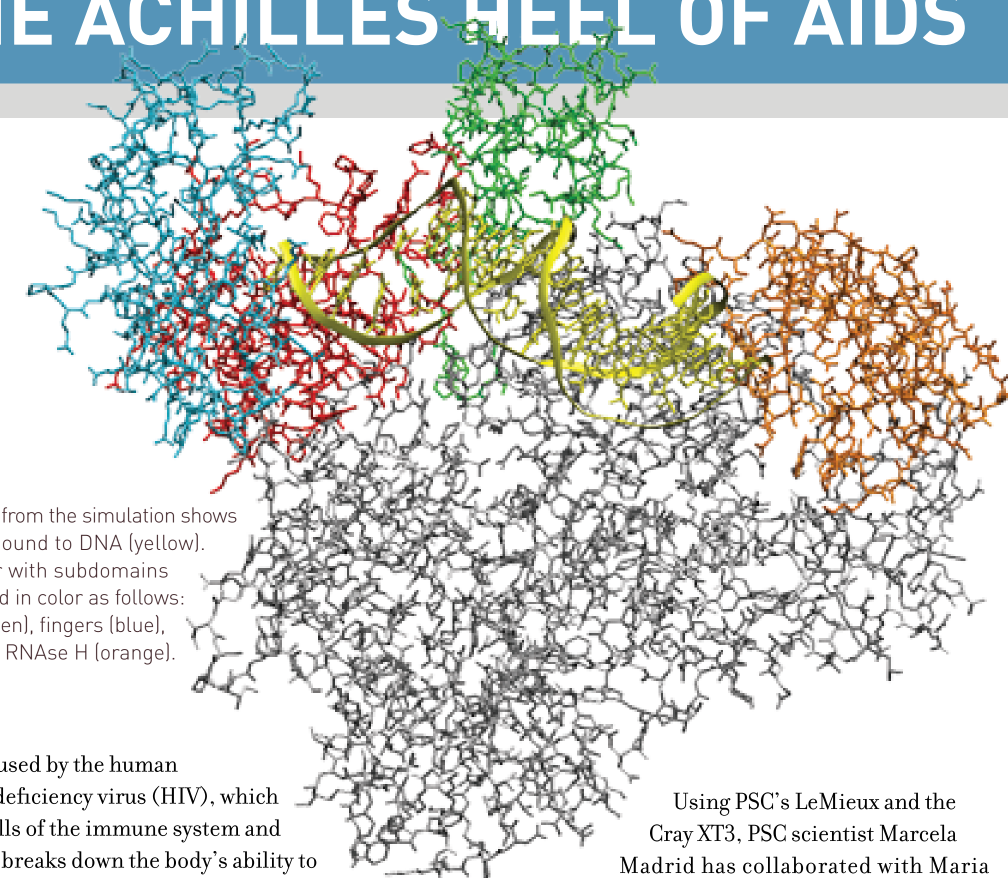
Over the past few years, Juri Toomre and graduate student Benjamin Brown at the University of Colorado, Boulder and Mark Miesch at the National Center for Atmospheric Research (NCAR) have used PSC's LeMieux and BigBen for very large-scale simulations of convection in the deep interior of stars. The convection patterns they model, known as giant cells, influence solar magnetic storms that can affect satellites and electrical systems on Earth.

In the solar interior, convection occurs as hot plasma rises and cooler, more dense plasma sinks. In this convection zone, from about 70-percent of the solar radius outward to the surface, scientists suspect that churning masses of plasma — giant cells — induce a global circulation pattern, moving plasma from the solar equator toward the poles near the surface, and then back to the equator at greater depth. This circulation generates magnetic fields that cause the 11-year sunspot cycle. Better understanding of this cycle and reliable prediction of associated solar storms would help to protect valuable assets in space and on Earth.

USING THE CRAY XT3 RESEARCHERS EXPLORE GIANT-CELL CONVECTION PATTERNS IN THE SUN

Using as many as 2,048 BigBen processors, the researchers modeled the sun's magnetism and internal rotation with a program they developed called ASH (Anelastic Spherical Harmonic). Terabytes of data produced by these simulations reside on disk storage at PSC, and the researchers analyze the data remotely via the TeraGrid network using software developed at NCAR called VAPOR. Their findings, forthcoming in the *Astrophysical Journal*, indicate that at low solar latitudes, plasma sinks along north-south corridors. At higher latitudes, rising and falling areas of plasma meet and create solar cyclones that last for days. "Understanding how stars build magnetic fields," says Miesch, "is a fundamental and enduring mystery that high-performance computing is helping to uncover."

THE ACHILLES HEEL OF AIDS



This image from the simulation shows HIV-1 RT bound to DNA (yellow). RT is silver with subdomains represented in color as follows: thumb (green), fingers (blue), palm (red), RNAse H (orange).

AIDS is caused by the human immuno-deficiency virus (HIV), which invades cells of the immune system and eventually breaks down the body's ability to fend off disease. HIV-1 reverse transcriptase (RT), a multi-functional protein that is part of HIV, essentially copies-and-pastes HIV's DNA, which is then incorporated into immune system cells of the infected person.

Interfering with RT's function would shut down HIV's reproductive capability, which explains why RT is the target of several FDA-approved anti-AIDS drugs.

DETAILED STUDIES OF HIV-1 RT COULD PROVIDE CLUES TO KNOCKING OUT AIDS

A precise, clear understanding of how RT works could make it possible to design more effective anti-AIDS drugs that could give a knockout punch to this worldwide scourge.

Using PSC's LeMieux and the Cray XT3, PSC scientist Marcela Madrid has collaborated with Maria Kurnikova and colleagues of Carnegie Mellon University to carry out molecular dynamics simulations of RT in the absence of DNA, as well as RT interacting with DNA. After long simulation times (beyond five nanoseconds), they observed that regions of RT that resemble the fingers and thumb of a hand tend to move apart — important for accommodating a large molecule like DNA. The DNA undergoes a "twist and slide" motion, which may facilitate its positioning at RT's active site. Interfering with this motion could disrupt RT's function. "This work will be important in drug design," says Madrid, "because it shows details of the motion that have not been observed before by any other computational technique."