Science AAAS

Modeling the Solar Dynamo

Paul Charbonneau and Piotr K. Smolarkiewicz

Science **340**, 42 (2013);
DOI: 10.1126/science.1235954

Struble *et al*. obtained convincing evidence for an organic fluoronium ion in solution by preparing a special polycyclic, cage-like precursor compound that provides steric protection to a fluoronium ion and limits possible decomposition and rearrangement pathways. To generate the fluoronium ion from this precursor, they used so-called solvolysis experiments, in which the precursor compound containing a leaving group (here a triflate group, -OTf) is heated in a suitable solvent (water or alcohols). Under these conditions, the leaving group is cleaved, which generates a short-lived cationic intermediate that is subsequently trapped by the solvent.

The analysis of the reaction products provides strong evidence for the intermediate generation of a fluoronium ion. In textbook-like nucleophilic substitution reactions, the substitution of the leaving group by the solvent should only occur at the carbon atom bearing the leaving group (by an S_N1 or S_N2 reaction) (see the figure, panel A). However, Struble *et al*. used isotopic labeling to show that substitution also occurs at the remote carbon where the fluorine was originally placed (panel B). Interestingly, direct and remote substitution is observed precisely in a one-to-one ratio, strongly indicative of a symmetrical, positively charged fluoronium intermediate.

The symmetrical structure of the fluoronium ion is further substantiated by high-level quantum-chemical calculation supporting a fluoronium structure as the actual reaction intermediate. In the structural formula, the charge is drawn at the fluorine (because of its hypervalent connection to two substituents), placing the positive charge at the most electronegative atom. However, the calculations reveal that the charge is largely located at the two carbon atoms next to the fluorine, resolving this contradiction.

The evidence provided by Struble *et al*. contradicts the current paradigm that organic fluoronium ions are too unstable to exist. Nevertheless, the fluoronium ion presented is only a short-lived reaction intermediate attested by indirect evidence. The direct observation of a fluoronium ion through spectroscopic techniques or x-ray crystallography is still pending and will most likely require the synthesis and isolation of more stable derivatives. The current report shows that this task should be possible if the fluoronium is embedded in a well-designed cage-like structure.

Although the fluoronium was only observed as a short-lived reaction intermediate, its observation could affect synthetic organofluorine chemistry. The formation of cyclic halonium ions as reaction intermediates is well attested for the other halogens and has had a lasting effect on the stereochemistry of halogenation reactions. Struble *et al*. show that, depending on the circumstances, formation of similar ions is also possible for organofluorine compounds. The use of tamed fluoronium ions as intermediates might enable new synthetic fluorination pathways for the synthesis of valuable organofluorine compounds.

Struble *et al*.'s results might also have wider implications in organofluorine chemistry. Because of its small size and its high electronegativity, fluorine's electrons are poorly polarizable, and organofluorine compounds generally interact with other atoms or molecules only through rather weak electrostatic interactions (*3*, *8*). It is usually assumed that more covalent interactions like the hypervalent bonding in the fluoronium generally do not occur, but taking into account these new results, this assumption might not be general.

References

1. P. Kirsch, *Modern Fluoroorganic Chemistry: Synthesis, Reactivity, Applications* (Wiley-VCH, Weinheim, Germany, 2004).
2. K. Uneyama, *Organofluorine Chemistry* (Blackwell, Oxford, UK, 2006).
3. D. O'Hagan, *Chem. Soc. Rev.* **37**, 308 (2008).
4. M. D. Struble, M. T. Scerba, M. Siegler, T. Lectka, *Science* **340**, 57 (2013).
5. V. Nguyen, X. Cheng, T. H. Morton, *J. Am. Chem. Soc.* **114**, 7127 (1992).
6. D. Mootz, K. Bartmann, *Angew. Chem. Int. Ed. Engl.* **27**, 391 (1988).
7. R. Panisch, M. Bolte, T. Müller, *J. Am. Chem. Soc.* **128**, 9676 (2006).
8. R. Berger, G. Resnati, P. Metrangolo, E. Weber, J. Hulliger, *Chem. Soc. Rev.* **40**, 3496 (2011).

10.1126/science.1236150

ASTRONOMY

Modeling the Solar Dynamo

Numerical simulations are changing our views on the dynamo process underlying the solar magnetic activity cycle.

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The Sun's magnetic field is the engine and energy channel underlying virtually all manifestations of solar activity. Its evolution takes place on a wide range of spatial and temporal scales, including a prominent 11-year cycle of successive polarity reversals over the entire star. This magnetic cycle in turn modulates the physical properties of the plasma flowing away from the Sun into interplanetary space, the frequency of all geoeffective eruptive phenomena (such as flares and coronal mass ejections), and the solar radiative flux over the full range of the electromagnetic spectrum—from x-rays through ultraviolet, visible, and infrared light, all the way down to radio frequencies (*1*). The Sun's heartbeat is truly magnetic, and recent numerical simulations (*2*–*5*) are providing new insights into its mode of operation.

Self-sustained amplification of a magnetic field through the action of fluid motions is called a dynamo. Dynamos operate through a physical effect called electromagnetic induction, discovered by Faraday in the 19th century. Induction is put to work in modern power-generating plants converting mechanical energy imparted to turbines (by water, wind, or steam) into electricity. There are no turbines inside the Sun, but in its outer third in radial extent, the so-called convection zone, mechanical energy abounds in the form of rotational shear and turbulent fluid motions driven by the solar luminosity. Plasma flowing across the magnetic field that pervades the solar interior induces electrical currents, which, under appropriate flow and magnetic field configurations, can sustain the field against dissipation. The magnetic field so generated in the solar interior subsequently emerges at the Sun's surface, structuring and energizing its extended atmosphere.

Parallel advances in raw computing power and ever more sophisticated numerical algorithms make it possible to produce and investigate magnetic cycles in Sun-like spheres of thermally convecting magnetized fluid. The underlying physics is in principle well understood in the form of magnetohydrodynamics (or MHD), being described by the classical fluid equations augmented by

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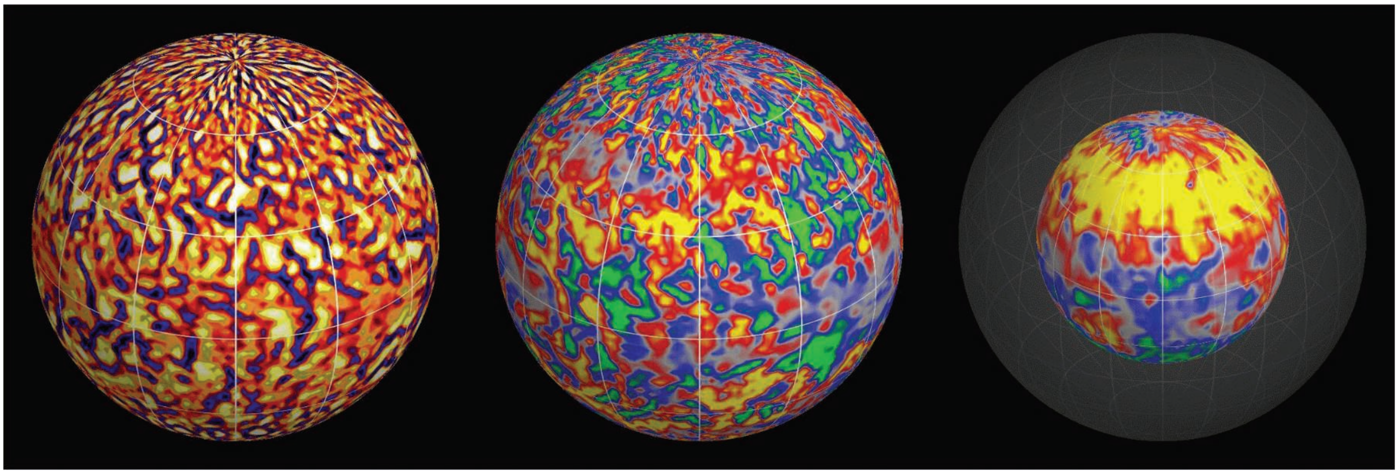
Published by AAAS



Solar simulations. Three snapshots of a magnetohydrodynamical numerical simulation of solar convection, carried out using the multiscale flow simulation model EULAG (*12*–*15*). The left panel shows a color rendering of the radial component of the convective flow (orange to light yellow, upflows; red to dark blue, downflows) in the subsurface layers of the simulation. The center panel shows the radial magnetic field (gray to yellow, outward-directed magnetic field; gray to green, inward-directed) at the same depth. Note how the characteristic spatial scales are the same for both quantities, which also evolve on the same temporal scale of days. The right panel shows the magnitude of the zonal magnetic field component, deep in the interior of the simulation, at the base of the convection layer. Note the banded structure at mid-latitudes, roughly symmetric about the rotation axis. This torus-like structure, and its opposite-polarity counterpart in the other hemisphere, undergo synchronous polarity reversals on a cadence of about 40 years.

Maxwell's laws of electromagnetism. The challenge lies with the strong nonlinearities characterizing the interactions of fluid flows and magnetic fields, as well as the extremely wide range of spatial and temporal scales over which these interactions take place under solar interior conditions.

Although the induction of intense magnetic fields by turbulent convection occurs readily in these numerical simulations [(*6*); (*7*) and references therein], it has proven much harder to establish the conditions allowing the self-organization of the spatiotemporally intermittent turbulent magnetic field into structures that maintain their spatial and temporal coherence over scales much greater than those of turbulent convection. The figure shows a snapshot of a simulation in which this self-organization has taken place. In the outer layers (left and center panels), the flow and magnetic field have roughly the same spatial scale; however, deep within the simulation domain (right panel), at the base of the turbulent convection layer, zonal bands of strong magnetic field are built up, parallel to and antisymmetric about the equatorial plane. This is precisely the type of internal magnetic field configuration believed to be conducive to the production of sunspots [(*8*) and references therein], the largest and most strongly magnetized structures found at the solar surface.

In the specific simulations displayed, the zonal magnetic field bands reverse their polarity quite regularly, every 40 years or so. This is longer than the observed solar cycle by a factor of ~4, but the very fact that a regular cycle is produced is already remarkable. Other numerical simulations, in principle quite similar in their overall design and parameter regimes, produce instead large-scale zonal structures within the turbulent convection layer, peaking at low latitudes, sometimes reversing their polarity on time scales of a few years, in other cases remaining steady. In these various simulations the internal flows are far more alike than the very different magnetic cycles emerging from their inductive action. Where the various simulation models differ is at the level of what one would normally hope to be details: grid resolution, the numerical treatment of dissipation at the smallest resolved scale, the presence of convectively stable fluid underlying the convecting layers. Evidently, something essential is hiding in these details.

If the Sun's large-scale magnetic field manages to remain quasi-steady on time scales much longer than that of convection, then a near-balance must exist between the inductive contributions of turbulent and large-scale flows (*9*, *10*), because dissipation is inefficient at these larger scales. The small residual induction is then what is driving the much slower cyclic evolution of the large-scale magnetic component (*11*). This delicate balance is most certainly influenced by the manner in which dissipation is implemented at the smallest spatial scales resolved in the simulations, and therein may lie some of the aforementioned sensitivity to "details." Other physical mechanisms that have received little attention may also be in play. Simulations similar to that shown in the figure (also see supplementary materials) reveal that accumulation of magnetic fields beneath the base of the convection zone may become prone to MHD instabilities triggered at those depths, which may in turn destabilize the cycle on very long time scales. Such instabilities may even play a role in timing the regular polarity reversals. Investigation of these mechanisms is a painstaking task, in view of the enormous volume of simulation data that must be stored, visualized, analyzed, and ultimately understood in physical terms. The real work is just beginning.

References and Notes

1. C. J. Schrijver, G. L. Siscoe, Eds., *Heliophysics, Vols. I, III and III* (Cambridge Univ. Press, Cambridge, 2010–2011).
2. M. Ghizaru, P. Charbonneau, P. K. Smolarkiewicz, *Astrophys. J.* **715**, L133 (2010).
3. P. J. Käpylä, M. J. Korpi, A. Brandenburg, D. Mitra, R. Tavakol, *Astron. Astrophys.* **548**, A88 (2010).
4. B. P. Brown, M. S. Miesch, M. K. Browning, A. S. Brun, J. Toomre, *Astrophys. J.* **731**, 69 (2011).
5. N. J. Nelson*et al*., *Astrophys. J.* **762**, 73 (2013).
6. F. Cattaneo, *Astrophys. J.* **515**, L39 (1999).
7. A. S. Brun*et al*., *Astrophys. J.* **614**, 1073 (2004).
8. Y. Fan, *Liv. Rev. Solar Phys* **6**, 4 (2009).
9. A. Hubbard, F. DelSordo, P. J. Käpylä, A. Brandenburg, *Mon. Not. R. Astron. Soc.* **398**, 1981 (2009).
10. B. P. Brown*et al*., *Astrophys. J.* **711**, 424 (2010).
11. É. Racine, P. Charbonneau, M. Ghizaru, A. Bouchat, P. K. Smolarkiewicz, *Astrophys. J.* **735**, 46 (2011).
12. www.mmm.ucar.edu/eulag
13. J. M. Prusa*et al*., *Comput. Fluids* **37**, 1193 (2008).
14. EULAG is used primarily in atmospheric and climate research. For its MHD extension, see (*15*).
15. P. K. Smolarkiewicz, P. Charbonneau, *J. Comput. Phys.* **236**, 608 (2013).

Supplementary Materials

www.sciencemag.org/cgi/content/full/340/6128/42/DC1

10.1126/science.1235954