ing directionality[10–13]. Thus, in both myosin and kinesin, the regions between the catalytic head and the adjacent stalk (the converter and neck, respectively) are important for specifying the direction of movement. And, although widely divergent in structure, these two regions seem to be functionally equivalent.

Now that a minus-end-directed myosin has arrived on the scene, and with the existence of minus-end-directed kinesins already well established, could the third class of linear motors, the dyneins, also have representatives that move in the other direction? All dyneins tested so far are minus-end-directed microtubule motors, but a provocative observation has come from studies of an exotic giant amoeba. In this cell, the kinetic and physiological properties of organelle movements along microtubules are characteristic of dynein going in both directions[14]. So, we may have to watch out for a backward-stepping dynein as well. ■

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Earth science

Taking the core temperature

Mark S. T. Bukowinski

The Earth's core extends from its centre to about 55% of Earth's radius, or about 2,900 km below our feet. And yet its effects on humanity are immense. The liquid outer core generates the Earth's magnetic field that shields us, and all other living things, from the solar wind. And by some estimates it provides sufficient heat to the bottom of the mantle to influence mantle convection and hence tectonic motions, earthquakes and volcanism. The extent of these and other influences depends on just how hot the core is relative to the mantle.

This is a matter that continues to challenge geophysicists, and is the subject tackled by Alfè *et al.* on page 462 of this issue[1]. The authors have applied new developments in computational physics to devise a virtual thermometer that may refine estimates of the temperature of the Earth's core. The technique involved is innovative and powerful, and should have much broader applications.

To appreciate the geophysical significance of Alfè and colleagues' contribution, consider first the temperatures in the Earth's mantle. Imagine going down a deep mine shaft. As you descend you start getting uncomfortably warm. Were you to go as deep as one kilometre, you would find that the temperature exceeds that at the surface by 20 to 30 °C. Vertical conduction along this temperature gradient is one mechanism by which the Earth rids itself of about 4.2×10^{13} joules of heat every second[2]. How does the temperature trend continue with depth and how much of the surface heat flow comes from the core?

Were the temperature to continue rising at a rate of 20 to 30 °C per kilometre, rocks would start vaporizing at a depth of a few hundred kilometres. However in most of the mantle heat is transported by highly efficient thermal convection, which reduces the gradient by two orders of magnitude. Only where vertical convective velocities are restricted by physical boundaries can a large thermal gradient arise. The boundary separating the silicate mantle from the iron-alloy core has a density contrast that is about twice that between the atmosphere and crust[3]. So any heat coming out of the core would form a thermal boundary layer at the bottom of the mantle. By estimating the concomitant temperature increase across the boundary, ΔT_{cm}, geophysicists would gain a valuable constraint on the total heat flux from the core, and insight into the core's physical and chemical properties.

Using geophysical, petrological and geochemical data, along with high-pressure experiments and geodynamic modelling, one can deduce that the temperature near the bottom of the mantle probably lies between 2,500 and 3,000 K (ref. 4). Estimates in the core rely on the assumption that the boundary between the solid inner core and the liquid outer core is at the melting temperature of the core material. Given that the core is made of iron with approximately 10% of lighter elements, and accounting for the fact that impurities tend to lower melting temperatures (although there is some evidence that oxygen in the core might increase melting temperature), a measurement of the melting temperature of iron at or near the pressure of the inner core boundary would probably place an upper bound on the core's temperature. Such estimates have been obtained by shock melting and by heating microscopic samples of iron in diamond-anvil high-pressure cells[5–9]. The measurements are difficult and their interpretation is controversial[10] — as shown in the 2,000 K

Box 1: *Ab initio* theory and the Earth

The chemical and physical properties of materials are described by quantum mechanics with great accuracy. However, for anything more complicated than the hydrogen atom, there are no exact solutions to Schrödinger's equation. The principal difficulty is the many-body nature of the problem, which is where density functional theory (DFT) comes in. This is based on the observation that the ground-state properties of materials are rigorously and uniquely determined by the one-electron density[13,14]. The many-body Schrödinger's equation is replaced by an equation with effective interactions that depend only on the electron density. Although the exact form of these effective interactions is not known, several approximations exist that yield very accurate structural and physical properties of molecules and condensed materials.

Ab initio DFT methods refer to calculations that rely on DFT but use no empirical information about the material. Given the atomic numbers of the constituent atoms, and known physical constants such as Planck's constant and electron charge, these calculations yield equilibrium structures, total energies, equations of state, vibrational frequencies and so on. Density functional theory has long appealed to geophysicists interested in understanding the physics of materials subjected to the extreme conditions in deep planetary interiors. Not surprisingly, the Earth's core was the early subject of such investigations[15]. Today DFT methods are being used successfully to examine the effects of pressure on the structure, elasticity and thermodynamics of complex silicates thought to make up the deep Earth[16,17].

Developments such as that described by Alfè *et al.* promise that it won't be long before *ab initio* methods will be used almost routinely to study such geochemical processes as partitioning of elements among coexisting phases, high-temperature and high-pressure phase transformations, and even the chemical reactions between core and mantle materials. **M. S. T. B.**

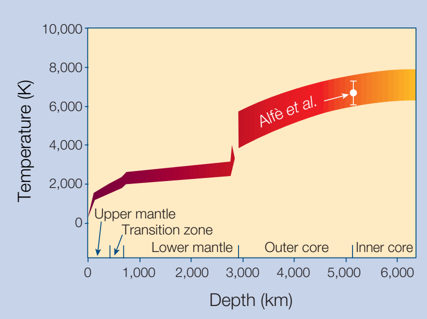

Figure 1 **Estimates of temperature inside the Earth. This geotherm — geophysicists' best estimate of the radial distribution of temperature — is known only imprecisely. The lines provide rough estimates based on a variety of geophysical, geochemical and laboratory data, helped by geodynamic simulations. There are two major boundary layers at the top and bottom of the mantle. There may also be another sharp increase in temperature at 660 km, the boundary between the lower mantle and the transition zone, if this boundary separates layers of distinct chemical composition. The geotherm is highly uncertain at the core–mantle boundary and within the core. Bounds within the core are based on the range of measured melting temperatures of iron. The circle with an error bar shows the estimated melting temperature of iron at the inner core boundary as calculated by Alfè *et al.*[1].**

span of temperatures that can be deduced from these experiments (Fig. 1).

Now a new player joins the quest. Alfè *et al.* use an *ab initio* molecular dynamics method[11] (Box 1), combined with a novel 'thermodynamic integration' scheme, to compute the free energies of solid and liquid iron as functions of pressure and temperature. By comparing these energies, they arrive at a melting curve that, the authors claim, competes in accuracy with existing experimental data. The calculated melting curve, which gives a temperature of 6,670 ± 600 K at the inner core boundary, is consistent with a calculation based on shock-wave data[5] and the diamond-anvil measurements of Williams *et al.*[6].

Alfè and colleagues' prediction leaves much uncertainty in the value of ΔT_{cm}. But the real significance of their contribution rests in its being the first completely *ab initio* calculation of the thermal properties of solid and liquid iron, and hence its melting curve, and the fact that its accuracy seems to be well supported by previous calculations of thermodynamic properties of solid and liquid iron. Other computations, for example those of Stixrude *et al.*[12], amply demonstrate the utility and credibility of *ab initio* theory. Nevertheless, only the future will tell whether the calculated iron melting curve is indeed accurate, just as it will tell which, if any, of the measured melting curves are accurate.

Meanwhile, this new study by Alfè *et al.* provides a benchmark for future computations and challenges the experimental community to try to converge on tighter limits on the melting temperatures. Further stimulus will probably come from computations of chemical potentials that should yield theoretical estimates of the solubility and thermal effects of sulphur, oxygen, hydrogen and other candidate alloying elements in the core. Such calculations should also allow estimates of the density change across the inner core boundary, as well as of the heat of fusion.

By combining *ab initio* computations with geophysical data it will then be possible to test the assumptions underlying the gravitational dynamo models: that the light component of the core is largely excluded from the inner core, leaving behind a buoyant residue that can drive convection in the outer core. The Earth can be thought of as a high-pressure experiment, a vast arena for the interplay of geophysical observation with experimental and computational materials science. For research, it is a clear win–win situation. ■

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Apoptosis

Cutting red-cell production

Stuart H. Orkin and Mitchell J. Weiss

For the proper delivery of oxygen to our tissues we need to have enough circulating red blood cells (erythrocytes). As Olympic officials have learned, artificially boosting the number of erythrocytes enhances athletic performance. But a potential downside of having excessive red blood cells is sluggish circulation and stroke. So, for good health, we need finely tuned regulation of red-cell production, and on page 489 of this issue DeMaria and colleagues[1] propose a new mechanism for how this might be accomplished.

The maturation of immature red-blood-cell precursors (proerythroblasts) into mature erythrocytes is positively controlled by a polypeptide hormone called erythropoietin, which promotes both proliferation and survival of erythroid precursors. The idea that the formation of red blood cells might also be negatively regulated has only recently been considered. In cell culture, binding of ligands to so-called death receptors on the surface of erythroid precursors activates death-promoting enzymes called caspases (cysteine proteases with aspartate specificity), and culminates in cell suicide (apoptosis). DeMaria and colleagues[1] now provide evidence that activation of death receptors on erythroid cells — or, alternatively, deprivation of erythropoietin — leads to caspase-induced cleavage (and, hence, inactivation) of a nuclear regulatory protein called GATA-1. This transcription factor is crucial for the maturation and survival of erythroid precursors. The authors' observations suggest a hitherto unknown negative-control mechanism by which life, death and cellular maturation decisions converge on a single protein target (Fig. 1, overleaf).

In mammals, red blood cells form in the bone marrow within anatomical units called erythroblastic islands. These units comprise macrophages (white blood cells that engulf foreign particles and microorganisms) surrounded by erythroblasts at different stages of maturation. The proliferation and survival of these erythroblasts depend on the presence of erythropoietin. Erythroblasts have erythropoietin receptors on their surface and, if deprived of erythropoietin, they succumb to apoptosis. In part, this reflects a requirement for signals from the erythropoietin receptor in inducing or stabilizing the expression of an anti-apoptotic protein called bcl-x_L (ref. 2). Indeed, as shown by a study of embryonic stem cells[3], bcl-x_L is also necessary for normal maturation of erythroid cells. So, as with many other types of cell, apoptosis must be held in check for normal development to ensue.

As well as extracellular anti-apoptotic signals, erythroblasts use internal programmes to ensure their own survival. The