CRUSTAL PERMEABILITY

Tom Gleeson and Steve Ingebritsen
Editors

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We dedicate this book to our families who support and inspire us, and to Henry Darcy whose legacy of solving both scientific and practical problems continues to guide the discipline of hydrogeology.

Conversion factors for permeability and hydraulic-conductivity units

In this book we emphasize the use of permeability (k) and SI units (m^2) as the measure of ease of fluid flow under unequal pressure. However hydraulic conductivity (K) and a variety of other units are used in practice. Permeability is a rock property, whereas hydraulic conductivity reflects both rock and fluid properties (fluid viscosity and density) – see Chapter 1. The approximate conversion from k to K here assumes that the fluid is water at standard temperature and pressure. Water viscosity varies by a factor of ~26 and water density by a factor of ~3 between 0° C and the critical point of water. Other fluids such as hydrocarbons can exhibit much larger viscosity ranges. In the table below, we show the unit conversion for 1 m^2 as well as 10^{-15} m^2 which is a more realistic permeability for geological materials.

		Permeability, k	Hydraulic conductivity, K		
	cm^2	Darcy	$m\ s^{-1}$	$m\ d^{-1}$	$ft\ d^{-1}$
$1\ m^2 =$	10^4	10^{12}	10^7	9×10^{11}	3×10^{12}
$10^{-15}\ m^2 =$	10^{-11}	0.001 (1 mD)	10^{-8}	9×10^{-4}	3×10^{-3}

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This book is accompanied by two companion websites:

One website includes:

- Powerpoints of all figures from the book for downloading

www.wiley.com/go/gleeson/crustalpermeability/

The other website includes:

- A persistent data portal for sharing crustal-permeability data

http://crustalpermeability.weebly.com/

CHAPTER 1

Introduction

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Permeability is the primary control on fluid flow in the Earth's crust. Thus, characterization of permeability is a central concern of many Earth scientists; hydrogeologists and petroleum engineers recognize it as their most essential parameter. More broadly considered, permeability is the key to a surprisingly wide range of geological processes, because it also controls the advection of heat and solutes and generation of anomalous pore pressures (Fig. 1.1). The practical importance of permeability – and the potential for large, dynamic changes in permeability – is highlighted by ongoing issues associated with hydraulic fracturing for hydrocarbon production ("fracking"), enhanced geothermal systems, and geologic carbon sequestration.

The measured permeability of the shallow continental crust is so highly variable that it is often considered to defy systematic characterization. Nevertheless, some order has been revealed in globally compiled data sets, including postulated relations between permeability and depth on a whole-crust scale (i.e., to approximately 30 km depth; e.g., Manning & Ingebritsen 1999; Ingebritsen & Manning 2010) and between permeability and lithology in the uppermost crust (to approximately 100 m depth: Gleeson *et al.* 2011). The recognized limitations of these empirical relations helped to inspire this book.

Although there are many thousands of research papers on crustal permeability, this is the first book-length treatment. Here, we have attempted to bridge the historical dichotomy between the hydrogeologic perspective of permeability as a static material property that exerts control on fluid flow and the perspective of economic geologists, crustal petrologists, and geophysicists who have long recognized permeability as a dynamic parameter that changes in response to tectonism, fluid production, and geochemical reactions.

This book is based in large part on a special thematic issue of the *Geofluids* journal published in early to mid-2015 (*Geofluids* **15**:1–2). Several changes and improvements differentiate the book from the thematic issue: the authors of the 22 original *Geofluids* papers have had the opportunity to revise and update their respective chapters, and three additional chapters have been added to fill gaps in the topical coverage (Ishibashi *et al.*, this book; Taron *et al.*, this book; Yardley, this book); the introductory material has been revised and expanded; the reference list has been consolidated and updated; an index has been added; and a complementary website (http://crustalpermeability.weebly.com/) has been built to house permeability data and other supporting information. Much of this introduction, and much of the bridging material between topical sections of the book, is derived from the introduction to the *Geofluids* thematic issue, with changes and additions where appropriate.

MOTIVATION AND BACKGROUND

This book is motivated by the controlling effect of permeability on diverse geologic processes; by practical challenges associated with emerging technologies such as hydraulic fracturing, enhanced geothermal systems, and geologic carbon sequestration; and by the historical dichotomy between the hydrogeologic concept of permeability as a static material property that exerts control on fluid flow and the perspective of other Earth scientists who have long recognized permeability as a dynamic parameter. Issues associated with hydraulic fracturing, enhanced geothermal systems, and geologic carbon sequestration have already begun to promote a constructive dialog between the static and dynamic views of permeability, and here we have made a conscious effort to include both viewpoints. We focus on the quantification of permeability, encompassing both direct measurement of permeability in the uppermost crust and inferential permeability estimates, mainly for the deeper crust.

The directly measured permeability (k) of common geologic media varies by approximately 16 orders of magnitude, from values as low as 10^{23} m^2 in intact crystalline rock, intact shales, and fault gouge, to values as high as 10^{-7} m^2 in well-sorted gravels. Permeability can be regarded as a process-limiting parameter in that it largely determines the feasibility of advective solute transport ($k \gtrsim 10^{-20}$ m^2), advective heat transport

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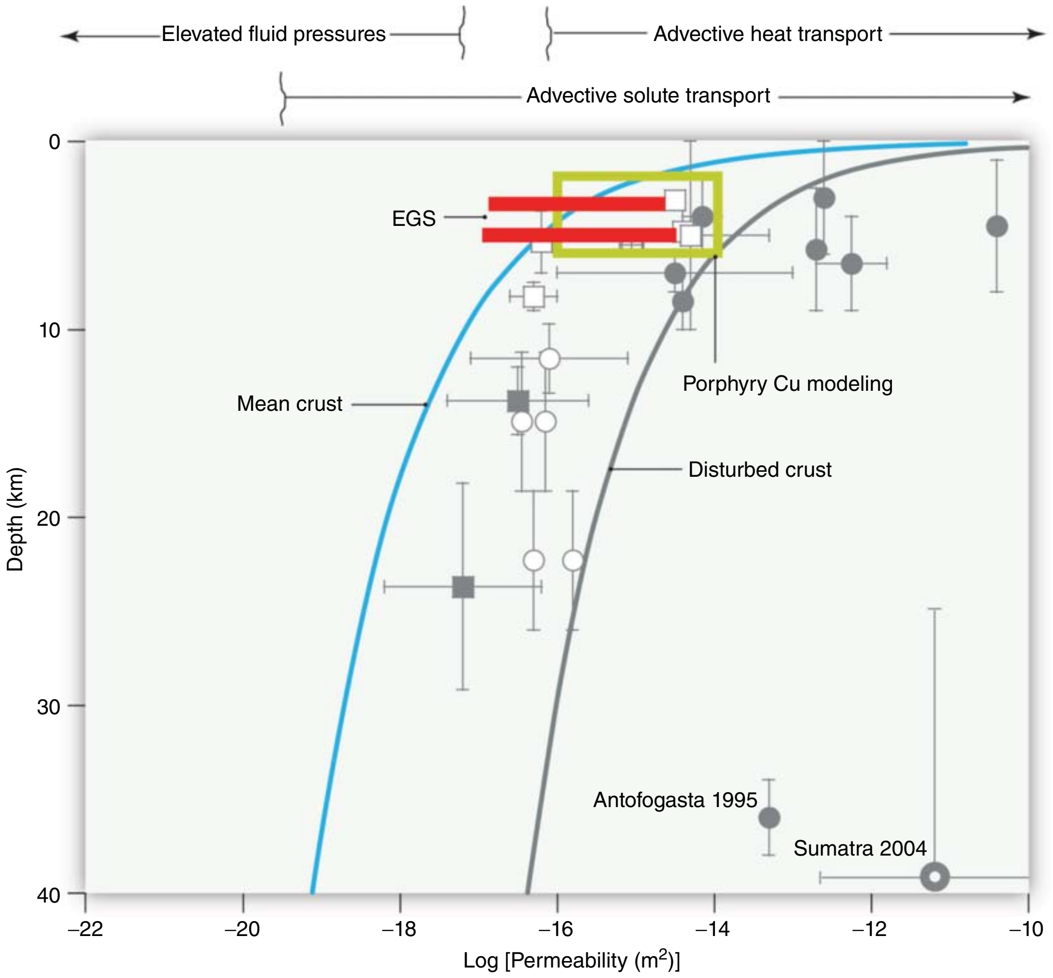

Fig. 1.1. Crustal-scale permeability (k) data. Arrows above the graph indicate approximate ranges of k over which certain geologically significant processes are likely. The "mean crust" k curve is based on k estimates from hydrothermal modeling and the progress of metamorphic reactions (Manning and Ingebritsen 1999). However, on geologically short timescales, k may reach values significantly in excess of these mean crust values (Ingebritsen and Manning 2010). The power-law fit to these high-k data – exclusive of the Sumatra datum (Waldhauser *et al*. 2012) – is labeled "disturbed crust." The evidence includes rapid migration of seismic hypocenters (solid circles), enhanced rates of metamorphic reaction in major fault or shear zones (open circles), recent studies suggesting much more rapid metamorphism than had been canonically assumed (solid squares), and anthropogenically induced seismicity (open squares); bars depict the full permissible range for a plotted locality and are not Gaussian errors. Red lines indicate k values before and after enhanced geothermal systems reservoir stimulation at Soultz (upper line) (Evans *et al*. 2005) and Basel (lower line) (Häring *et al*. 2008) and green rectangle is the k-depth range invoked in modeling the formation of porphyry-copper ores (Weis *et al*. 2012). (*See color plate section for the color representation of this figure.*)

($k \gtrsim 10^{-16}\,\mathrm{m}^2$), and the generation of elevated fluid pressures ($k \lesssim 10^{-17}\,\mathrm{m}^2$) (Fig. 1.1) – processes which in turn are essential to ore deposition, hydrocarbon migration, metamorphism, tectonism, and many other fundamental geologic phenomena.

In the brittle upper crust, topography, magmatic heat sources, and the distribution of recharge and discharge dominate patterns of fluid flow, and externally derived (meteoric) fluids are common (e.g., Howald *et al.*, this book). In contrast, the hydrodynamics of the ductile lower crust are dominated by devolatilization reactions and internally derived fluids (e.g., Connolly & Podladchikov, this book). The brittle–ductile transition between these regimes occurs at 10–15 km depth in typical continental crust. Permeability below the brittle–ductile transition is non-negligible, at least in active orogenic belts (equivalent to mean bulk k of order 10^{-19} to $10^{-18}\,\mathrm{m}^2$) so that the underlying ductile regime can be an important fluid source to the brittle regime (e.g., Ingebritsen & Manning 2002).

The objective of this book is to synthesize the current understanding of static and dynamic permeability through representative contributions from multiple disciplines. In this introduction, we define crucial nomenclature, discuss the "static" and "dynamic" permeability perspectives, and very briefly summarize the contents of the book. Additional summary and synthesis can be found before and after the three main sections of the book, which are labeled "the physics of permeability," "static permeability," and "dynamic permeability."

NOMENCLATURE: POROSITY, PERMEABILITY, HYDRAULIC CONDUCTIVITY, AND RELATIVE PERMEABILITY

Here, we define some of the key hydrogeologic parameters that are repeatedly used in this book, namely porosity, permeability, hydraulic conductivity, and relative permeability. These are conceptually related but distinct concepts.

First, we note that all of these parameters are continuum properties that are only definable on a macroscopic scale. Perhaps most obviously, at any microscopic point in a domain, porosity ($V_{\text{void}}/V_{\text{total}} = n$) will be either 0 in the solid material or 1 in a pore space. As one averages over progressively larger volumes, the computed value of n will vary between 0 and 1 and, if the medium is sufficiently homogeneous, the volume-averaged value of n will eventually become nearly constant over a volume range, which has been termed the representative elementary volume (REV) (Bear 1972, 1979). Figure 1.2 shows, for example, a hypothetical section of volcanic ash-flow tuff; note the distinctly different porosity of the flow center relative to the flow top and bottom.

The concept of permeability – the ability of a material to transmit fluid – also applies only at an REV scale and can be regarded as reflecting detailed solid–fluid geometries that we cannot map and thus wish to render as macroscale properties. Exact analytical expressions for permeability can be obtained for simple geometries such as bundles of capillary tubes or parallel plates (constant-aperture fractures), but actual pore-fracture geometries are never known.

Porosity (n)–permeability (k) relations have been the subject of many studies (e.g., Luijendijk & Gleeson, this book), and there is often a positive correlation between these two essential quantities. However, even in the case of classical porous media, a correlation between n and k cannot be assumed for mixed-size grains, or when comparing media with greatly different grain sizes. For instance, although there is a positive correlation between n and k for clays themselves, clays are 10^4–10^{10} times less permeable than well-sorted sands (e.g., Freeze & Cherry 1979), despite having generally higher porosities. Furthermore, positive correlation between n and k cannot be assumed in more complex media. Consider again our ash-flow tuff example (Fig. 1.2): the top and bottom of an ash flow cool relatively rapidly, retaining their original high porosities (approximately 0.50), but the permeability of this “unwelded” material is relatively low, because the pores are small and not well connected. If the ash flow is sufficiently thick, pores deform and collapse in the slowly cooling interior, where the final value of porosity can be quite low (<0.05). However, the flow interior also tends to fracture during cooling, and the interconnected fractures transmit water very effectively despite the low overall porosity. The net result of the cooling history is that flow interiors typically have up to 10^4 times higher permeability than “unwelded” flow tops and bottoms, despite their much lower porosities (0.05 vs. 0.50).

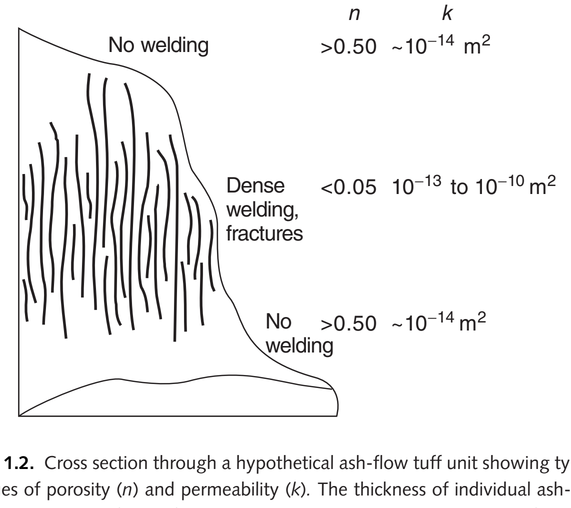

Fig. 1.2. Cross section through a hypothetical ash-flow tuff unit showing typical values of porosity (*n*) and permeability (*k*). The thickness of individual ash-flow tuff sheets ranges from a few meters to more than 300 m. Tertiary ash-flow tuffs are widespread in the western United States, particularly in the Basin and Range province. (Adapted from Winograd 1971.)

Both laboratory and *in situ* (borehole) testing normally return values of hydraulic conductivity (K) rather than permeability (k), and this parameter reflects both rock and fluid properties:

$$K = \frac{k\rho_f g}{\mu_f},$$

where $\rho_f g$ is the specific weight of the fluid and μ_f is its dynamic viscosity. In order to compare rock properties among different geothermal conditions, or different fluids (e.g., hydrocarbons vs. aqueous fluids), it is necessary to convert measured values of K to values of k (e.g., Stober & Bucher, this book). Considering once again our ash-flow tuff example: if the surficial outcrop depicted in Figure 1.2 could somehow be translated from standard temperature and pressure (STP = 15°C, 1 bar) to 300°C and approximately 1000 bars (approximately 10 km depth), without any changes in its physical morphology, its permeability k would not change, but its hydraulic conductivity would be approximately 10 times larger because of the increase in the ρ_f/μ_f ratio.

Finally, the empirically based concept of relative permeability is used to extend the linear flow law for viscous fluids (i.e., Darcy’s law) to multiphase systems. Relative permeability (k_r) represents the reduction in the mobility of one fluid phase due to the interfering presence of another fluid phase in the pore space and is treated as a scalar varying from 0 to 1, usually as some function of volumetric fluid saturation (e.g., $V_{\text{liquid}}/V_{\text{void}}$, where for instance $[V_{\text{vapor}} + V_{\text{liquid}}]/V_{\text{void}} = 1$). This concept is widely invoked in the context of hydrocarbon migration and production (oil–gas–liquid water) and unsaturated flow above the water table (air–liquid water), but is also applied to multiphase flow in hydrothermal systems – for instance by Weis (this book), who allows for the presence of three distinct phases in the void space (vapor + liquid + solid NaCl). Because methane-saturated shales can have very low permeabilities to basinal brines, some studies have used relative permeability effects to explain anomalous pressure in mature sedimentary basins (e.g., Deming *et al.* 2002).

STATIC VERSUS DYNAMIC PERMEABILITY

Some economic geologists, geophysicists, and metamorphic petrologists have long recognized permeability as a dynamic parameter that changes in response to dewatering, fluid production, and seismicity (e.g., Sibson *et al.* 1975; Walder & Nur 1984; Yardley 1986; Hanson 1995; Connolly 1997). For the purposes of this book, we consider "dynamic permeability" to include any transient variation in permeability, regardless of timescale. However, as pointed out by Huber & Su (this book), "dynamic permeability" also has a traditional and much narrower technical definition as frequency-dependent permeability.

The view of permeability as a dynamic parameter varying with time is in stark contrast to the hydrogeologic concept of permeability as a static material property that exerts control on fluid flow. Indeed, the term "intrinsic permeability," widely used in the hydrogeologic and petroleum engineering literature, seems to imply an immutable property.

However, there is abundant evidence that permeability varies in time as well as space, and that temporal variability in permeability is particularly pronounced in environments characterized by strong chemical and thermal disequilibrium. Laboratory experiments involving hydrothermal flow in crystalline rocks under pressure, temperature, and chemistry gradients often result in order-of-magnitude permeability decreases over daily to subannual timescales due to water–rock interaction (e.g., Morrow *et al.* 1981; Moore *et al.* 1994; Yasuhara *et al.* 2006), and field observations of continuous, cyclic, and episodic hydrothermal-flow transients at various timescales also suggest transient variations in permeability (e.g., Baker *et al.* 1987; Hill *et al.* 1993; Haymon 1996; Fornari *et al.* 1998; Sohn 2007). The occurrence of active, long-lived (10^3–10^6 years) hydrothermal systems (Cathles *et al.* 1997), despite the tendency for permeability to decrease with time due to water–rock interaction, implies that other processes such as hydraulic fracturing and earthquakes regularly create new flow paths (e.g., Rojstaczer *et al.* 1995). Indeed, in the past decade, coseismic permeability enhancement and subsequent permeability decay have been directly observed (Elkhoury *et al.* 2006; Kitagawa *et al.* 2007; Xue *et al.* 2013). It is also clear that sufficiently overpressured fluids cannot be contained in the crust and will create the permeability necessary to escape (e.g., Cathles & Adams 2005; Connolly & Podladchikov 2015; Weis, 2015). These various observations have inspired suggestions that crustal-scale permeability is a dynamically self-adjusting or even emergent property (e.g., Townend & Zoback 2000; Rojstaczer *et al.* 2008; Weis *et al.* 2012), reflecting a dynamic competition between permeability creation by processes such as fluid sourcing and tectonic fracturing and permeability destruction by processes such as compaction, diagenesis, hydrothermal alteration, and retrograde metamorphism. An important caveat is that there is likely a fundamental difference between permeability structure and evolution between prograde and retrograde metamorphism (Yardley, this book). Whereas pervasively wet rocks and near-lithostatic fluid pressures may accompany prograde metamorphism, localized hydration of dry rocks by fluid flow under near-hydrostatic fluid pressures is likely characteristic of retrograde metamorphism.

CONTENTS OF THIS BOOK

The following chapter of this book proposes a data structure to embrace and extend the existing knowledge of crustal permeability. The remainder of this book can be broadly categorized as dealing with the physics of permeability (5 chapters), static permeability (6 chapters), and dynamic permeability (13 chapters). Additional summary and synthesis sections are provided before and after these three main sections of the book.

DATA STRUCTURES TO INTEGRATE AND EXTEND EXISTING KNOWLEDGE

We live in an era of exploding information technology. Thus, the initial chapter in this book, by Fan *et al.*, outlines a vision for the "DigitalCrust": a community-governed, four-dimensional data system of the Earth's crustal structure. The DigitalCrust concept calls for a particular emphasis on crustal permeability and porosity, which have not been synthesized elsewhere and play an essential role in crustal dynamics. The Crustal Permeability data portal associated with this book at http://crustalpermeability.weebly.com/ is a complementary effort intended to unearth permeability data currently tucked away in many dusty corners of the web and in even dustier reports, books, and theses. The intent is to provide links to online, peer-reviewed permeability data that are globally accessible. In contrast to DigitalCrust, the Crustal Permeability data portal will not host data, and data do not have to be spatially located. Data requirements are simply that the data be peer reviewed (published in a peer-reviewed journal, book, or report); include permeability or other related fluid flow and transport parameters; and be hosted and publicly available on an online data repository such as figshare or institutional web pages such as the those of the United States Geological Survey (USGS).

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CHAPTER 2

DigitalCrust – a 4D data system of material properties for transforming research on crustal fluid flow

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ABSTRACT

Fluid circulation in the Earth's crust plays an essential role in surface, near-surface, and deep-crustal processes. Flow pathways are driven by hydraulic gradients but controlled by material permeability, which varies over many orders of magnitude and changes over time. Although millions of measurements of crustal properties have been made, including geophysical imaging and borehole tests, this vast amount of data and information has not been integrated into a comprehensive knowledge system. A community data infrastructure is needed to improve data access, enable large-scale synthetic analyses, and support representations of the subsurface in Earth system models. Here, we describe the motivation, vision, challenges, and an action plan for a community-governed, four-dimensional data system of the Earth's crustal structure, composition, and material properties from the surface down to the brittle–ductile transition. Such a system must not only be sufficiently flexible to support inquiries in many different domains of Earth science, but it must also be focused on characterizing the physical crustal properties of permeability and porosity, which have not yet been synthesized at a large scale. DigitalCrust is envisioned as an interactive virtual exploration laboratory where models can be calibrated with empirical data and alternative hypotheses can be tested at a range of spatial scales. It must also support a community process for compiling and harmonizing models into regional syntheses of crustal properties. Sustained peer review from multiple disciplines will allow constant refinement in the ability of the system to inform science questions and societal challenges and to function as a dynamic library of our knowledge of Earth's crust.

Key words: data integration, deep-crustal dynamics, earth system models, groundwater, groundwater–surface water interaction, permeability

MOTIVATION

Fluid flow in the Earth's crust depends strongly on material permeability, which varies in space and through time. As data and knowledge accumulate, and as we increasingly tackle interdisciplinary questions (Bodnar *et al.* 2013), a georeferenced, time-evolving data system of crustal structure and properties is needed to address a wide range of scientific and societal questions.

Understanding Earth's critical zone

The Earth's critical zone is the region from the top of the terrestrial biosphere to the depth of active groundwater circulation

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Companion Websites: www.wiley.com/go/gleeson/crustalpermeability/
http://crustalpermeability.weebly.com/

(National Research Council 2001). Critical zone science focuses on understanding the physical, chemical, and biological processes regulating critical zone evolution, determining its role in sustaining human society and terrestrial ecosystems, and predicting responses to anthropogenic, climatic, and tectonic forcing (Banwart *et al.* 2013). Fluid circulation plays a central role in critical zone processes, regulating chemical weathering, soil formation, ecosystem evolution, and biogeochemical cycling (Berner & Berner 1996; Jones & Mulholland 2000; Brantley *et al.* 2011; Boano *et al.* 2014). Carbon cycle research has focused on the Earth's atmosphere and surface, but 99.9% of all carbon is stored in the lithosphere (Kempe 1979). Thus, even small changes in fluxes from the crust can have major consequences for the ocean–atmosphere system. Chemical weathering, a primary driver of global biogeochemical cycling, depends strongly on subsurface water residence times (Berner 1978; Maher & Chamberlain 2014), which is primarily controlled by 3D hydrological flow paths and material rock properties (McGuire *et al.* 2005). Weathering depth is unknown (West 2012) yet critical to understanding global biogeochemical fluxes. Existing predictions of material fluxes are based on 2D bedrock geological maps and, therefore, neglect deeper rock strata and geothermal waters (e.g., Becker *et al.* 2008). A major advance in overcoming these and many other limitations would be a 4D knowledge system for managing and synthesizing existing and newly acquired data on the Earth's crust.

Assessing resource sustainability

Groundwater is the largest freshwater resource and primary source of drinking water for two billion people (Morris *et al.* 2003a). It also plays a central role in agriculture (Foster & Chilton 2003; Giordano 2009) and sustains the health of many ecosystems (Alley *et al.* 2002). Nevertheless, groundwater is not adequately managed to ensure sustainability (Danielopol *et al.* 2003; Foster & Chilton 2003; Brunner & Kinzelbach 2005; Konikow & Kendy 2005; Fogg & LaBolle 2006; Gleeson *et al.* 2010; Sophocleous 2010), and nearly a quarter of humanity lives in areas of groundwater stress (Gleeson *et al.* 2012a). A key factor in sustainability is groundwater residence time related to the renewal rate, which can be many millennia, well beyond the typical time horizon of human policies (Gleeson *et al.* 2012b). Residence time has been modeled assuming a consistent decrease in permeability with depth (Jiang *et al.* 2010b), but a single low permeability layer can control groundwater age (Gassiat *et al.* 2013).

Fluid hydrocarbons in the upper crust also currently play a vital role in the energy budget for society. Knowledge of subsurface structures and properties is a prerequisite for addressing many of the energy issues surrounding energy resources, including harvesting of geothermal energy (Mortensen & Axelsson 2013), carbon sequestration (Shrag 2007; Benson & Cole 2008), exploitation of unconventional oil/gas reservoirs, and fluid-injection-induced seismicity associated with all of these activities (Hitzman *et al.* 2012).

Understanding deeper crustal dynamics

Hydrogeologists, geologists, and geophysicists have begun to actively explore the role of groundwater and other subsurface fluids in fundamental geologic processes, such as crustal heat transfer, ore deposition, hydrocarbon migration, seismicity, tectonic deformation, and diagenesis and metamorphism (e.g., Burns *et al.* 2015; Connolly & Podladchikov 2015; Howald *et al.* 2015; Micklethwaite *et al.* 2015; Miller 2015; Okada *et al.* 2015; Weis 2015). The permeability of the Earth's crust is of particular interest because it largely determines the feasibility of important physicochemical processes, such as advective solute/heat transport (Burns *et al.* 2015; Saffer 2015) and the generation of elevated fluid pressures by processes such as physical compaction, heating, mineral dehydration, and fluid injection (Connolly & Podladchikov 2015; Miller 2015; Weis 2015).

Current understanding supports a general distinction between the hydrodynamics of the brittle upper crust, where hydrostatic fluid pressures are the norm and meteoric fluids are common, and those of the ductile lower crust, where metamorphic reactions and internally derived fluids dominate hydrodynamic behavior. The brittle–ductile transition between these regimes depends on temperature, strain rate, and rheology, but occurs at 10–15 km depth in typical continental crust. In tectonically active regions, high permeability episodically exists below the brittle–ductile transition (Connolly & Podladchikov 2015), such that fluid input from the ductile regime can be important to the cycling of some elements, and perhaps even to the balancing of the global water cycle over geologic time (Ingebritsen & Manning 2002).

This book highlights the historical dichotomy between the hydrogeologic concept of permeability as a static material property that exerts control on fluid flow and the perspective of other Earth scientists who have long recognized permeability as a dynamic parameter that changes in response to tectonism, devolatilization, and geochemical reactions. The dynamic view of crustal permeability is consistent with indications that fluid pressure is close to the lithostatic load during prograde metamorphism below the brittle–ductile transition (e.g., Fyfe *et al.* 1978); sufficiently overpressurized fluids cannot be contained in the crust, leading to fracturing and other processes that create permeability. More recently, it has been suggested that the permeability of the brittle crust may also be dynamically self-adjusting, responding to tectonism and external fluid sources much as the deeper crust responds to the magnitude of internal fluid sources (cf., Cathles & Adams 2005; Rojstaczer *et al.* 2008; Weis *et al.* 2012). The temporal evolution of permeability can be abrupt or gradual: stream-flow responses to moderate-to-large earthquakes demonstrate that dynamic stresses can instantaneously change permeability by factors of up to 20 on a regional scale, whereas a 10-fold decrease in the permeability of a package of shale in a compacting basin may require 10^7 years (Ingebritsen & Gleeson 2015). Thus, in the absence of seismicity, assuming that permeability is a static parameter can be reasonable for low-temperature hydrogeologic investigations with timescales of days to decades. Data compilations of deeper crustal material properties are likely to lead to a markedly better understanding of deeper crustal dynamics.

Supporting earth system modeling

There is an urgent need for large-scale data synthesis to support the development of integrated earth system models, which account for material and energy fluxes and key abiotic–biotic interactions in the atmosphere, lithosphere, and hydrosphere. Earth system models are critical tools for predicting future global environmental change, such as that addressed by the Intergovernmental Panel on Climate Change. However, even well-understood groundwater–surface water interactions in the top tens of meters of the crust are poorly represented in current earth system models, and most do not include subsurface processes at depths >2–3 m. Efforts to extend earth system models deeper into the crust have been hindered by deficiencies in subsurface data. Global, realistic 3D gridded permeability and porosity fields for continental crust do not yet exist, but recent efforts to map near-surface permeability and porosity (Gleeson *et al.* 2014) provide an important starting point.

DATA INTEGRATION TO TRANSFORM SCIENCE

Table 2.1 is a partial list of ongoing data integration efforts that have impacted our views of Earth systems interactions in many different ways. One example is the Macrostrat database (Peters 2006), which integrates existing stratigraphic information and aims to represent the Earth's upper crust as surface polygons that extend from the surface downward as stacks of lithostratigraphic and chronostratigraphic units. Macrostrat has integrated more than 36,000 rock units in North America, New Zealand, and the deep sea and is being augmented with the DeepDive machine reading system (Peters *et al.* 2014). Interactions between biotic and abiotic processes leave signatures in the rock record, and Macrostrat puts these signatures back into stratigraphic context, allowing them to be quantified in a space–time framework. Fossil records in the Paleobiology Database and the GPlates paleogeographic reconstructions are integrated with these data to produce a 4D model of the evolving Earth. Global-scale, deep-time syntheses of biological, geochemical, and sedimentary data have allowed new quantitative tests of long-standing hypotheses. For example, large-scale

Table 2.1 Examples of ongoing data integration efforts and the starting point of DigitalCrust

Data	Source	Format
World Topography, Bathymetry	CSDMS: http://csdms.colorado.edu/wiki/Topography_data	Gridded
FAO World Harmonized Soil Map	IIASA: http://webarchive.iiasa.ac.at/Research/LUC/External-World-soil-database/HTML/	Global gridded, polygons for countries
Global Lithologic Map	University of Hamburg: http://www.clisap.de/research/b:-climate-manifestations-and-impacts/crg-chemistry-of-natural-aqueous-solutions/global-lithological-map/	Surface polygons
World Geologic Maps	USGS WMS and ESRI map services: http://energy.usgs.gov/OilGas/AssessmentsData/WorldPetroleumAssessment/WorldGeologicMaps.aspx	Surface polygons
World Tectonic Stress Map	GFZ Potsdam: http://dc-app3-14.gfz-potsdam.de/pub/introduction/introduction_frame.html	Gridded, with points and lines
Global Sediment Thickness	UCSD: http://igppweb.ucsd.edu/~gabi/sediment.html	Gridded
Global Map of Surface Heat Flow	Map: Cardiff U: http://onlinelibrary.wiley.com/doi/10.1002/ggge.20271/abstract, Point: IHFC: http://www.heatflow.und.edu/	Gridded and points
National Geothermal Data System, SMU Geothermal Map	http://geothermaldata.org/, http://www.smu.edu/Dedman/Academics/Programs/GeothermalLab/DataMaps	Gridded maps and points, thermal profiles, thermal conductivity
Continental Stratigraphy	University of Wisconsin: http://macrostrat.org/. Data set of polygons tessellating North America, with associated time-stratigraphy description	Polygons with vertical sequence of layers
Global Aquifer Maps	BGR and UNESCO: http://www.whymap.org/whymap/EN/Home/whymap_node.html	Surface polygons
US Aeromagnetic Survey	USGS: http://mrdata.usgs.gov/magnetic/	Gridded, resolutions vary from region to region
US Gravity Anomaly	USGS: http://mrdata.usgs.gov/geophysics/gravity.html	Gridded
Groundwater Atlas, 25 US Aquifers	USGS: http://pubs.usgs.gov/ha/ha730/gwa.html	Surface polygons with thickness (isopachs)
Global Permeability and Porosity	McGill University (GLHYMPS): http://onlinelibrary.wiley.com/doi/10.1002/2014GL059856/abstract	Surface polygons

compilations of sedimentary data have played an important role in modeling biogeochemical cycling (e.g., Ronov 1978; Berner 2004), and Macrostrat has been used to calibrate sulfate burial fluxes and to better constrain the role of the sulfur cycle in regulating atmospheric oxygen (Halevy *et al.* 2012; Canfield & Kump 2013). Spatial–temporal patterns of sedimentation in Macrostrat have also been shown to quantitatively reproduce many major features in the macroevolutionary history of marine animals (Peters 2005, 2008b; Finnegan *et al.* 2011) and planktonic foraminifera (Peters *et al.* 2013). Combined with stable isotopic proxy records of biogeochemical cycling, global temperature, and rates of volcanism and crustal weathering, it appears likely that the correlations between paleobiological and macrostratigraphic data reflect common biological and stratigraphic responses to Earth system changes (e.g., Peters 2005; Hannisdal & Peters 2011), a hypothesis that emerges from, and can only be adequately tested with, integrated data deriving from the Earth's crust.

A second example is the UN-FAO Global Harmonized Soil Database. Large amounts of soil survey data from multiple nations and continents, often built using different soil taxonomies, horizon definitions and attributes, and compiled at different scales of resolution and with different formats, were harmonized through an international partnership, which defined a new set of soil attributes critical to agriculture and recommended methodologies for developing taxo-transfer rules. The result was a global data set at 30 arc-sec grids with 20 soil physical, chemical, and biological attributes. This data set (and predecessors) has been the sole basis for deriving soil hydraulic parameters necessary for calculating soil water fluxes in all global land models and servers as the primary resource for constraining global soil organic carbon stocks and fluxes (e.g., Batjes 1996; Hiederer & Kochy 2011).

THE DIGITALCRUST VISION

We envision a 4D space–time (*xyz–t*) data infrastructure designed to accommodate the structure and properties of the upper crust, from the surface down to the brittle–ductile transition, which occurs at 10–15 km depth in continental crust with a geothermal gradient of ~25–30°C km^{-1} but can be as shallow as 4–5 km in regions of high heat flow. In regions with adequate seismic networks, the brittle–ductile transition can be crudely mapped on the basis of the distribution of earthquakes with depth (e.g., Nazareth & Hauksson 2004; Tanaka & Ishikawa2005).

DigitalCrust must be a web-oriented, data-service-enabled, and spatially and temporally referenced workspace where the geosciences community can contribute and register data and model outputs, visualize, explore, and synthesize existing data to test hypotheses across space–time in ways that account for uncertainties. This is a daunting task and will require support from the broader Earth science community, including from initiatives such as EarthScope, national and regional geologic surveys, and funding agencies. Later, we describe some of the key elements required in DigitalCrust.

A geologic scaffolding

The foundation of DigitalCrust is a geologic scaffolding that describes the basic geologic fabric of the Earth's upper crust, from the critical zone to the brittle–ductile transition, and includes data spanning its full range of physical, chemical, and biological properties (Fig. 2.1). To accomplish this, DigitalCrust must receive contributions from all disciplinary domains involving the lithosphere, the hydrosphere, and the biosphere. Thus, despite the fact that it was originally motivated by the need to better understand and model crustal fluid flow, it must be an integrative data infrastructure that spans multiple domains of expertise in the Earth sciences. This broad vision is an attempt both to express the actual level of Earth systems integration that we believe occurs in nature and to respond to a common scientific and data infrastructure need that has been expressed in many Earth science communities. Because the most relevant intersection for many different types of geoscientists is defined by the common field location and rocks that they work on, regardless of whether or not they share any scientific expertise or disciplinary knowledge, DigitalCrust stands to promote both data discovery and interdisciplinary cross-fertilization by proactively connecting scientists on the basis of their intersection in the Earth's crust.

Hydrogeologic properties as key data content and service

Within the foundational geologic scaffolding, DigitalCrust will support multiscale integration of fluid-relevant properties. Improved description and synthesis of these properties, particularly permeability and porosity, have been a driving force behind DigitalCrust. Although millions of soil and aquifer analyses and measurements have been made, the data are dispersed and unstructured in the scientific literature, government archives, and myriad online web pages and repositories. Scales, standards, and formats also vary. We face several major challenges, including discovering this vast amount of information and organizing it within the geologic scaffolding and developing automated methods and algorithms for deriving meaningful hydrogeologic properties based on multiple data types.

Community knowledge repository and management system

As a community knowledge repository, DigitalCrust will integrate existing large-scale data sets (e.g., Table 2.1) and leverage current visualization tools to allow scientists to view what data already exist at given *xyz–t* coordinate and within a domain context, and what data/knowledge gaps remain to be filled. It will then allow scientists to contribute data sets to the growing knowledge base through a DigitalCrust node, with support for placing the data in an archival repository, obtaining an identifier

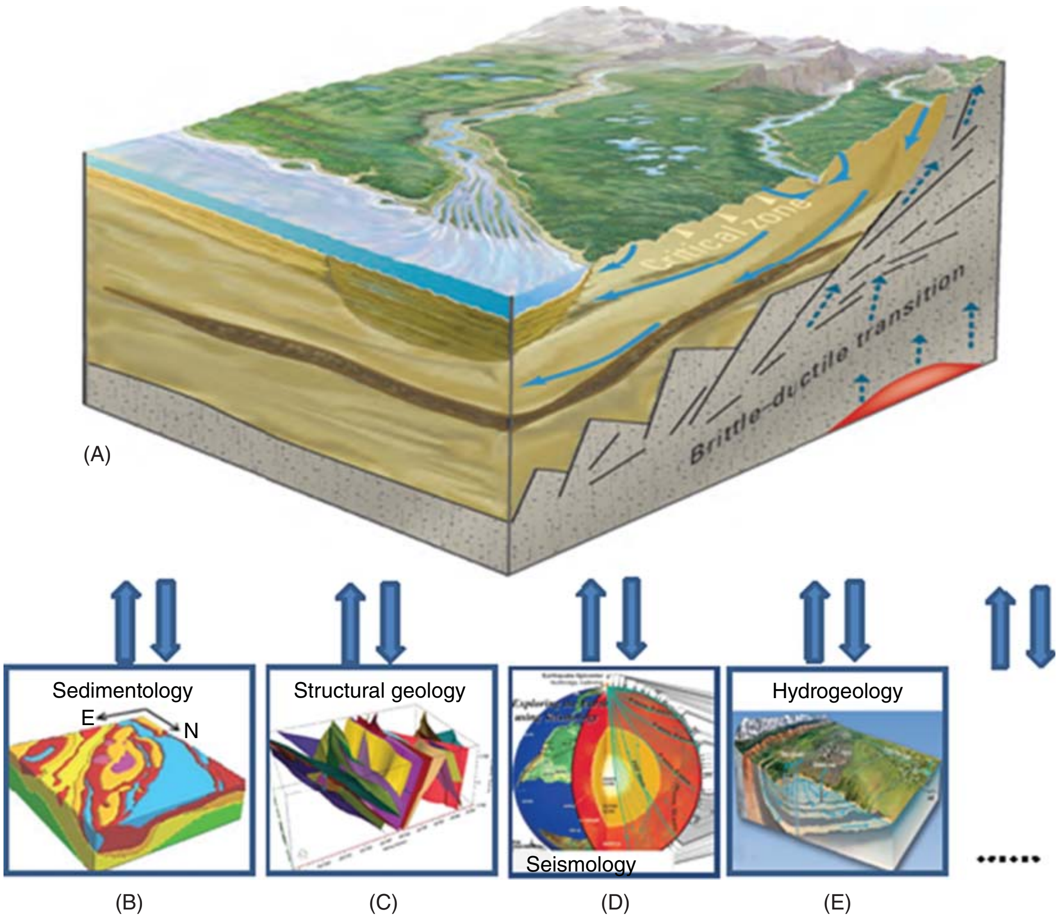

Fig. 2.1. The geologic scaffolding of DigitalCrust from the critical zone to the brittle–ductile transition (A), receiving contribution from and delivering service to a wide range of Earth science disciplines (B–E). (Image source: (A) Adapted from Winter *et al*. (1998), (B) McInerney *et al.* (2005), (C) Hinz *et al.* (2012), (D) IRIS (http://www.iris.edu/hq/), and (E) Paschke *et al.* (2011)). (*See color plate section for the color representation of this figure*.)

for data, and releasing it for community use. Contributors can view how their new entries fit into or impact the framework and receive a response from the system with recommendations on related data that they may not be aware of, as well as recognition of their data/knowledge contribution.

As a knowledge management system, DigitalCrust will index geoscience data sources from raw observation, through multiple levels of processing, interpretation, integration, and synthesis into models that are also incorporated into the repository. Linkage between observations and derived data sets through this chain should allow tracing provenance of information. The system should also include tools for social interactions such as review, discussion, correction, and updates to observations and interpretations at all levels. The resources in this system are accessed using simple web protocols and interchange formats that are documented, tested, and adopted by the DigitalCrust community. The data/information at a given geographic reference point will be delivered via an open application programming interface (API) that will support the development of specialized third-party applications as well as the DigitalCrust online resource itself.

Central to the vision is the use of a branching and versioning system, such as "Git" and "GitHub" in software development, which supports a common repository of best available data and most proven models, while allowing any researcher to create their own development fork. Formal peer review and community consensus will integrate branches back into the master DigitalCrust branch. Borrowing from the genomics community, which allows microcitation to unambiguously reference discrete data on organisms (Patrinos *et al.* 2012), DigitalCrust will provide a capacity for citing and referencing data and data products.

Given the anticipated scope, DigitalCrust must be governed by the community it intends to serve. It differs from many common crowdsourcing models in that contributions will be attributed to specific members of the scientific community, allowing the community to regulate itself by, for example, trusting or not trusting the contributions based on individually demonstrated knowledge and expertise. A community