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Swiss Journal of Geosciences

ORIGINAL PAPER

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SAPHYR: Swiss Atlas of Physical Properties of Rocks: the continental crust in a database

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Abstract

The Swiss Atlas of Physical Properties of Rocks (SAPHYR) project aims at centralize, uniform, and digitize dispersed and often hardly accessible laboratory data on physical properties of rocks from Switzerland and surrounding regions. The goal of SAPHYR is to make the quality-controlled and homogenized data digitally accessible to an open public, including industrial, engineering, land and resource planning companies as well as governmental and academic institutions, or simply common people interested in rock physics. The physical properties, derived from pre-existing literature or newly measured, are density, porosity and permeability as well as seismic, magnetic, thermal and electrical properties. The data were collected on samples either from outcrops or from tunnels and boreholes. At present, data from literature have been collected extensively for density, porosity, seismic and thermal properties. In the past years, effort has been placed especially on collecting samples and measuring the physical properties of rock types that were poorly documented in literature. A workflow for quality control on reliability and completeness of the data was established. We made the attempt to quantify the variability and the uncertainty of the data. The database has been recently transferred to the Federal Office of Topography swisstopo with the aim to develop the necessary tools to query the database and open it to the public. Laboratory measurements are continuously collected, therefore the database is ongoing and in continuous development. The spatial distribution of the physical properties can be visualized as maps using simple GIS tools. Here the distribution of bulk density and velocity at room conditions are presented as examples of data representation; the methodology to produce these maps is described in detail. Moreover we also present an exemplification of the use of specific datasets, for which pressure and temperatures derivatives are available, to develop crustal models.

Keywords: Physical properties, Continental crust, Database, Density, Seismic velocity

1 Introduction

Physical properties of rocks are key parameters for several Earth Science disciplines spanning from oil industry to engineering, geophysics, petrology, structural geology and water resources. They provide the essential link between observed geophysical data and interpreted geology. Measurements of rock properties have been performed over many decades by numerous laboratories to support various investigations into the structure and composition of the Earth. For Switzerland, in particular, data collection of physical properties has been facilitated by the presence of mountain chains over a large part of the national territory, which offers access to a vast variety of rock types of different age, origin and composition. The Swiss Atlas of Physical Properties of Rocks (SAPHYR) unifies this information into a single data base (dbase) structure and makes it accessible to everyone. This dbase is thus aimed for usage by different scientific disciplines as well as by industry and the public.

SAPHYR is a representative dbase containing the major physical properties of rocks, with full coverage for continental crustal rocks. We take advantage of the rich rock
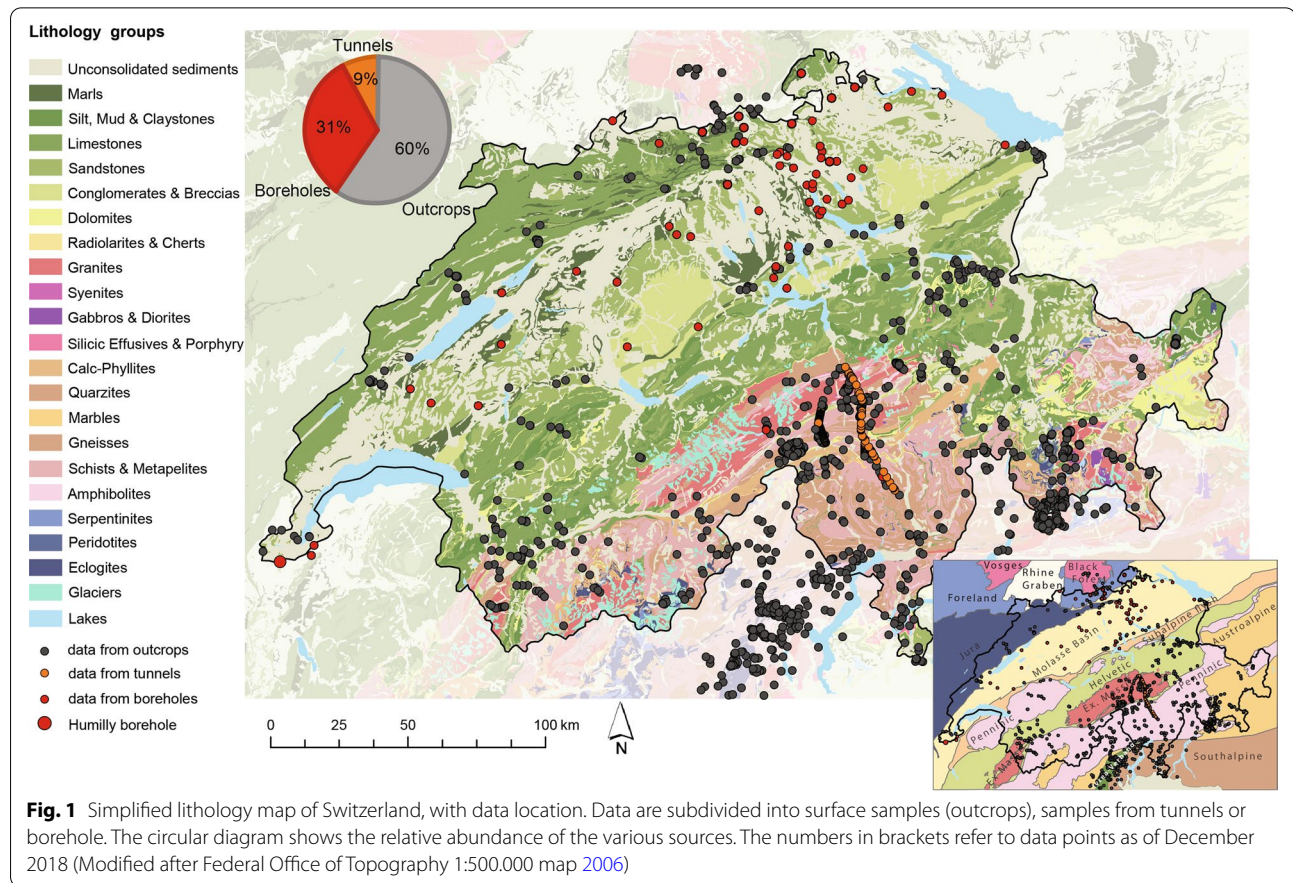

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assembly presented by the Swiss Alps and their forelands, including the Ivrea-Verbano Zone (Pfiffner, 2014; Quick et al., 2003) towards South and the Black Forest and Vosges Massifs towards North. The term "representative" underlines our aims to (1) represent all major crustal lithologies with an emphasis on shallow crustal layers (sediments), and to (2) assess a complete suite of the most important physical properties of rocks.

The digital geotechnical map of Switzerland version 1/2000 at scale 1:500.000(GK500) issued by the Federal Office of Topography (2006) in cooperation with the Swiss Geotechnical Commission (SGTK), has been chosen as basis for our dbase because it provides lithological description of the rock types we address, and depicts their occurrence in outcrops. The dbase is, therefore, strongly "rock type" oriented. The starting point of the data collection has been the detection and recognition of main rock types on the basis of mineral composition and texture representing the main components of a mature Phanerozoic continental crust (Christensen & Mooney, 1995; Hawkesworth et al., 2010).

The majority of the properties in the SAPHYR dbase

with data of samples from boreholes and tunnels. A limited amount of data (mainly for thermal properties) has been obtained by various labs on cuttings from tunnel and borehole samples. In Fig. 1 the three different sources of samples, outcrop, boreholes, and tunnels are distinguished. The physical properties we address are density, ultrasound seismic properties (compressional and shear waves), magnetic susceptibility, thermal conductivity, heat production, porosity and permeability, and when applicable their anisotropy. We consider this dataset an almost complete characterization of the physical identity of each rock type representing the continental crust. The distribution of the data points (sample locations) is illustrated in Fig. 1.

At each step in the development of the dbase we performed an assessment on the representative significance and quality of the sample assembly, we kept track of the measurement methodologies and measurement uncertainties and whenever possible we investigated the dependence of physical properties on environment conditions (pressure, temperature and other). Each procedure step in data collection and manipulation was

Fig. 1 Simplified lithology map of Switzerland, with data location. Data are subdivided into surface samples (outcrops), samples from tunnels or borehole. The circular diagram shows the relative abundance of the various sources. The numbers in brackets refer to data points as of December 2018 (Modified after Federal Office of Topography 1:500.000 map 2006)

are measured on samples from outcrops and combined

documented in order to guarantee a full transparency at

each stage and to allow further discussion on the quality and relevance of data and procedures. The main target is to reach a scientifically solid product fully transparent in its derivation with easy access for public usage. In addition to our own measurements and to the published data, where possible we analysed and integrated industry data collections generally not publicly available and usually un-discussed for relevance and quality. Figure 2 illustrates the main procedural steps in the compilation of the dbase and the visualization of its content.

We chose to organize our data in the form of a geographically referenced dbase. We adopted a geographic information system (GIS) to store our data because it is the most convenient system to manipulate, analyse, manage, and present geographical and spatial data. A GIS provides an ideal spatial data infrastructure for our data, that are essentially geographic data (linked to the location where the samples or the boreholes are located), allowing to implement a framework of geographic data, metadata, and tools that are interactively connected, therefore it permits to use and represent our spatial data in an efficient and flexible way. Moreover we took advantage of the already established geological and tectonic GIS available for Switzerland that fully covers the whole national territory (Federal Office of Topography, 2006; https://www.eea.europa.eu/data-and-maps/data/eea-reference-grids-2/gis-files/switzerland-shapefile).

SAPHYR has been conceived and supported by the Swiss Commission of Geophysics following and extending an earlier study by Wagner et al. (1999). With SAPHYR we aim to provide a dbase of physical properties of all major continental crustal rock types, and to collect derivatives with pressure and temperature, where possible, in order to allow extrapolation of the physical properties to burial condition at depth. A major focus was to collect as much as possible data from rock types representative of all continental crustal levels and their heterogeneities (Best, 1995; Hacker et al., 2015; McLennan, 1995; Rudnick, 1992; Sobolev & Babeyko, 1989), though not necessarily abundant in outcrops. For example, ultramafic rocks outcrop in limited areas, but they are important components of the lowermost part of the crust. Therefore, data on those rocks have been specifically collected too, taking care to sample a variety of ultramafic rocks. We decided to present each data as a single data point linked to geographical coordinates either of the rock specimens or of the boreholes in the case of data collected in deep wells. In the latter case, additional information such as boreholes identification data (owner, date of perforation, max depth reached, geological formation at bottom well), stratigraphy and depth at which the data were collected are also presented.

We also decided to visualize the surface distribution of the main physical properties (density and velocity of compressional waves) on the basis of the rocks outcropping within and in the vicinity of Switzerland. In such case, the products are presented (Fig. 2) as maps of Switzerland with contoured and color-coded values of the specific property. The statistical data treatment and the processing of the specific physical properties, that brought to the drawing of the "rock physics" maps is described in the next sections.

2 The SAPHYR data compilation
### 2.1 The sources
The data that populate our dbase have four distinct sources: scientific literature, public reports from industry or governmental institutions, unpublished data of various sources (upon agreement by original authors), and, most important, a great number of new laboratory measurements specifically obtained for this dbase (Fig. 3).

The information has been compiled in two separate parts of the dbase. One part contains data from outcrops and tunnels and the other data from boreholes. The decision to separate the data is based on the consideration that samples from outcrops and tunnels usually denote one data per latitude/longitude and are characterized by an exhumation history of the area, which might affect most of the physical parameters. At the same time the depth at which data from boreholes are collected is in itself a parameter that need to be taken into consideration. Data from boreholes are limited to lab measurements on core samples retrieved from boreholes. No log-based data were included in the dbase, because we considered the two kinds of data not directly comparable. In fact for borehole logging data, the support volume of these kinds of measurements tends to be one to two orders of magnitude larger than that of typical lab measurements.

The starting point for data collection has been an extensive screening of the relevant, mostly international, scientific literature of the last 40 years of laboratory data on rocks from Switzerland and surrounding regions. Most of the literature data derives from peer reviewed papers containing sample's description and location, experimental methodology statement, and measurements of physical properties. A list of the literature that was screened and contained data suitable for the SAPHYR dbase is reported in Additional file 1. At present we screened the viable scientific literature published from 1976 to 2019. The data from such literature amounted to about 40% of the dbase (see Additional file 1: S1 "dbase data literature"). In a second phase we screened Ph.D. and Master theses, monographs, academic review works, public technical reports from the various governmental
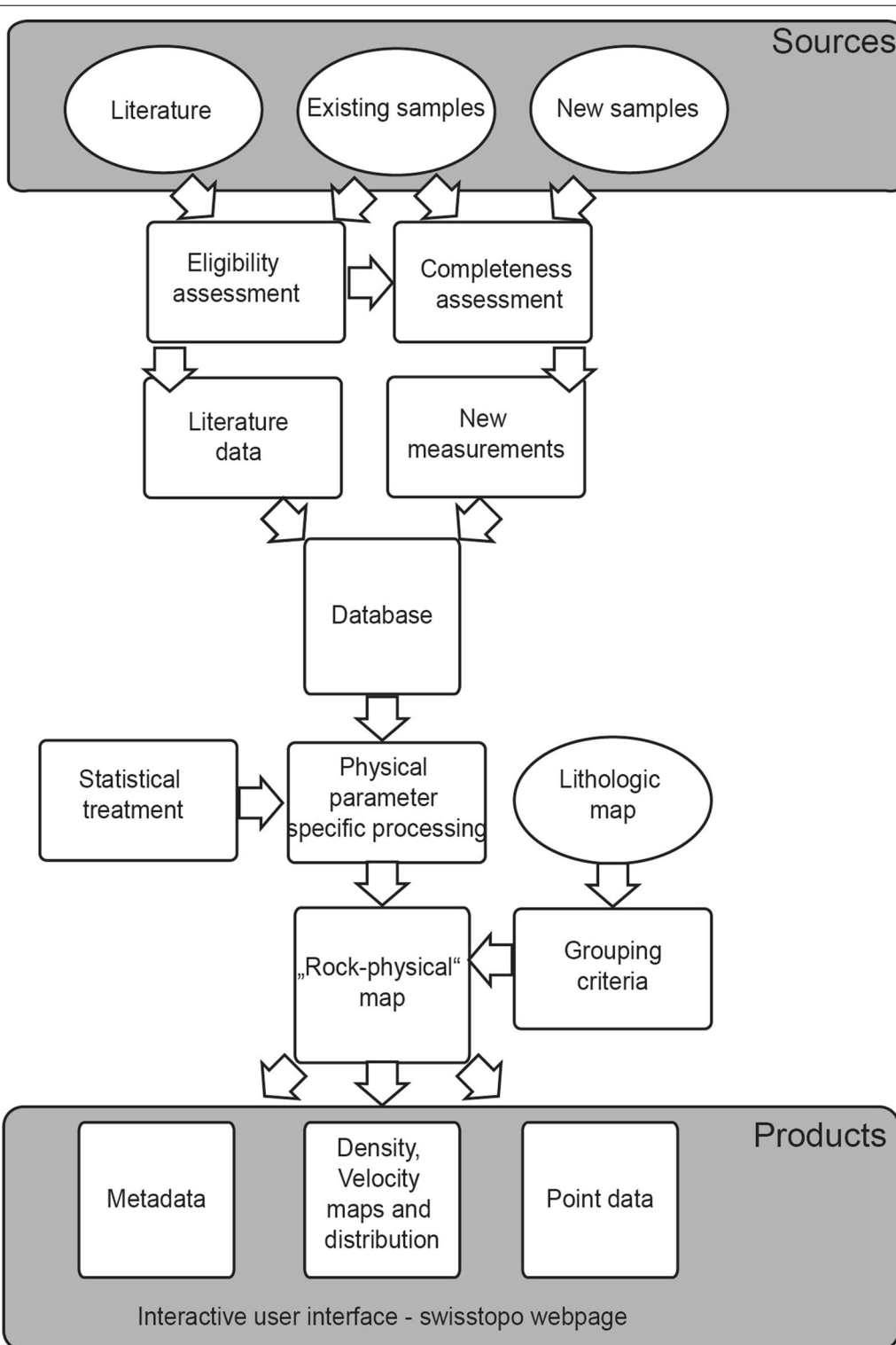
Fig. 2 General structure of the methodology applied to establish the SAPHYR dbase is illustrated in this flow chart. The procedure that leads from the sources to the products has been based on a scientific approach of evaluation of data quality and errors, together with traceability of data sources. Statistical procedures have been applied to evaluate the state of completeness of our dataset and to define the appropriate values characterizing rock types (see text)
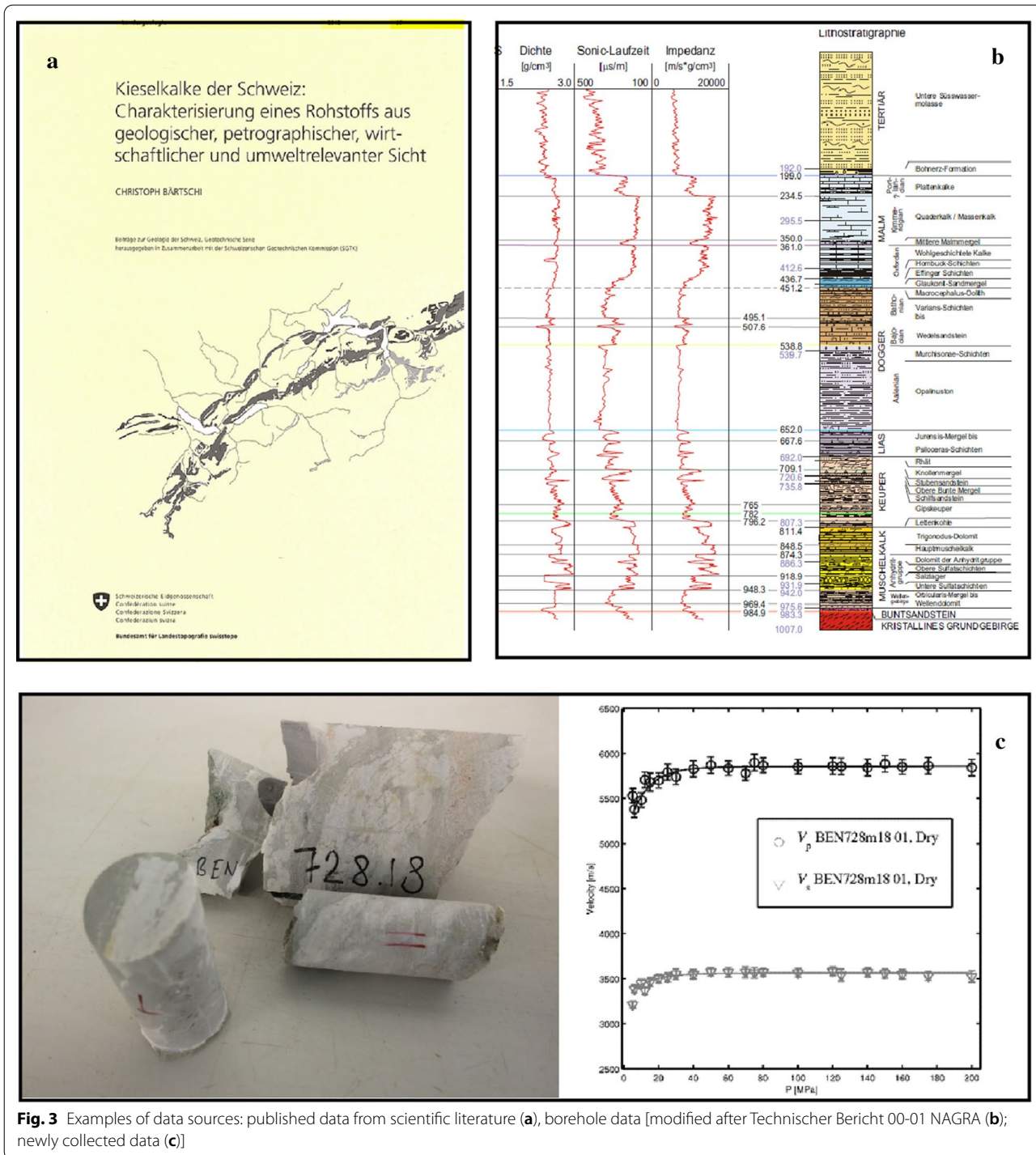
Fig. 3 Examples of data sources: published data from scientific literature (**a**), borehole data [modified after Technischer Bericht 00-01 NAGRA (**b**); newly collected data (**c**)]

agencies such as NAGRA (the National Technical Competence Centre for deep geological disposal of radioactive waste), from the Swiss Commission of Geophysics itself and the Swiss Geotechnical Commission, incrementing the data collection by about 30%. The oldest publication in this group dates back to 1936 while the youngest dates from 2015. Unpublished proprietary data from private laboratories and consultants offices in the fields of geology, underground water, geothermal exploration and geophysics have been collected and included in the dbase upon agreements on intellectual properties of the data. They represent a minor percentage in the

data collection, and the data of such sources are mainly used for statistical treatments. Moreover those data have been admitted in our collection only if the experimental methodology used was documented to conform with the scientific methods and after an adequate evaluation of the data quality.

A sample collection of 261 cores from the Institute of Geophysics of ETH Zurich on which thermal properties had been previously measured, were made available to us for further laboratory investigation. The cores were suitable for density, porosity, magnetic properties and velocities measurements. Magnetic susceptibility has been measured on the same cores and the data acquired during this campaign accounts for more than 50% of the whole magnetic data collection of the dbase. Figures 3 and 4 illustrate data sources and their proportion in the dbase.

After screening the available literature (see Additional file 1: S1 "dbase data literature") and after acquitting additional physical properties on the already available sample collections (as described in Sect. 4), new data acquisition campaigns were promoted in those cases where the data population was considered insufficient to represent either a specific geographic area, or a specific rock type (see Additional file 1: S2 "lithology list"). In particular, the sediments underlying the Swiss Molasse basin needed targeted investigation and this was performed acquiring about 40 new samples from boreholes and from outcrops.

In every case, before starting new field campaigns in order to further sample those lithologic and tectonic units that were under-represented, we considered performing new measurements on rock samples already available from previous studies, where the size of the samples and their preservation condition were sufficiently good. We aimed to collect as many physical properties as possible on the same samples. In case of anisotropic properties, if structural planes and directions were recognizable and if the sample dimension allowed, measurements were performed on cores cut from the same sample along the main structural directions (for more details see Additional file 1: S3 "anisotropic parameter measurements").

We underline that literature data, public, scientific or semi-private, up to now constitutes the majority in
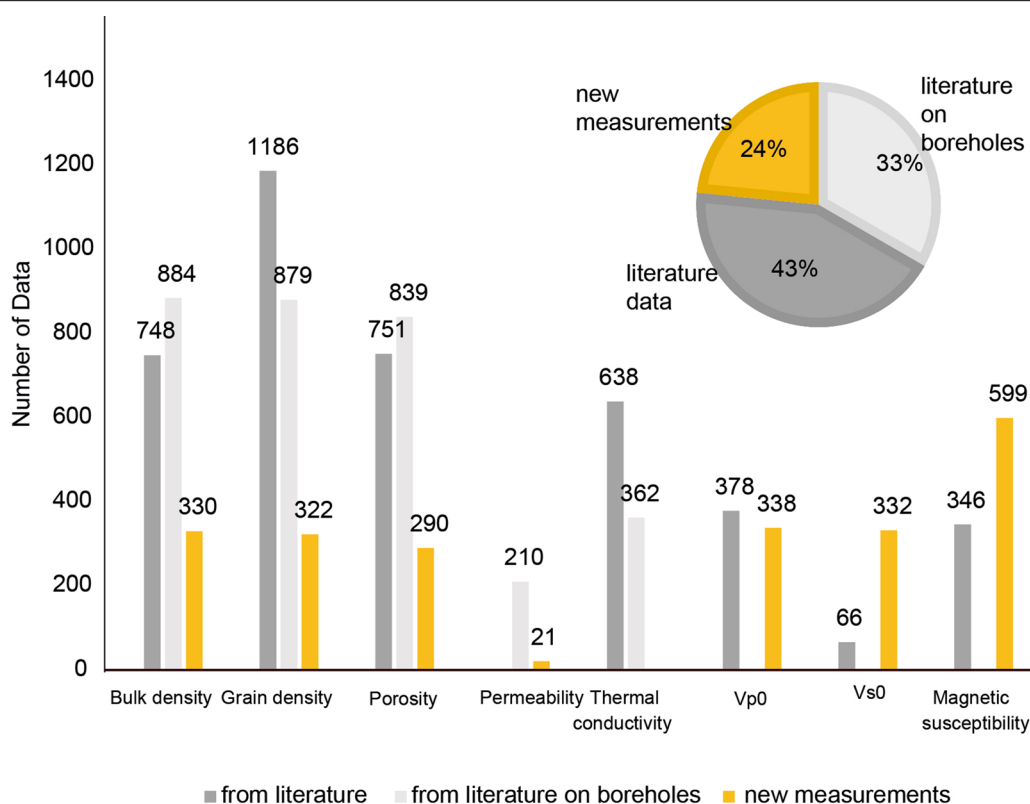
Fig. 4 Proportion of the different data sources. In term of absolute number of data, the main source is literature (scientific literature, public reports, industrial technical reports, Ph.D. theses, and other). In this figure we differentiate data from boreholes as explained in the text; almost all the borehole data derive from NAGRA public reports. Note that for some specific properties the contribution of the new measurements has been significant, as, f.e., for magnetic susceptibility. The numbers refer to data as of December 2018

our dbase, and data from own new measurements represent only 24%. Nevertheless, for some specific properties, the new measurements represent a significant contribution (i.e., magnetic properties and ultrasound shear velocities).

2.2 Physical properties

The physical properties collected are density and porosity, thermal properties, magnetic properties and ultrasound velocities (Table 1). All data units are expressed in International System of Units.

The commonly used methods reported in literature for physical rock parameter measurements are briefly presented in Sect. 3.2, while a detailed description of the

methods used to perform new measurements of physical properties is given in Sect. 3.3.

2.3 The samples: representative sampling of rocks

The data we collected derive in great majority from outcrops, tunnels and boreholes in Switzerland. A list of rock types that we considered representative of all components of a typical continental crust is reported in the Additional file 1: S2 "lithology list". Rocks from the Swiss Alps are mostly representative of upper to middle crust, due to the structural evolution and exhumation mechanisms, with successive erosion of the Alpine orogenic wedge. The lowermost levels of the continental crust are represented with a broad variety of rock types

Table 1 Physical properties collected in the SAPHYR database

Physical parameters	Units	Symbol	Condition
Density		ρ	
Bulk	g/cm^3		Dry/saturated
Grain	g/cm^3		Dry/saturated
Porosity		φ	
Absolute	%		
Open total[a]	%		
Open macro-[a]	%		
Open micro-[a]	%		
Permeability		κ	
Absolute	md		
Anisotropy	%		
Thermal properties			
Thermal conductivity	W/mK	λ	Dry/saturated
Specific heat capacity	J/kgK	c	Dry/saturated
Conductivity anisotropy	%		
Heat production			
^{238}U, ^{235}U, ^{232}Th, ^{40}K content	ppm		
Volumetric heat generation	μW/m^3	A	
Magnetic properties			
Bulk susceptibility	m^3/mol	K	
Anisotropy (Kmax/Kmin)			
Deviation factor P	m^3/mol	ΔK	
Seismic properties			
Ultrasound velocity of P waves	km/s	Vp	Dry, room pressure and temperature
Vp pressure derivative	km/sK	$\Delta_p - Vp$	High pressure
Vp temperature derivative	km/sMPa	$\Delta_T - Vp$	High temperature
Vp recalculated at room pressure[b]	km/s	Vp_0	Dry, room pressure and temperature
Ultrasound velocity of S waves	km/s	Vs	Dry, room pressure and temperature
Vs pressure derivative	km/sMPa	$\Delta_P - Vs$	High pressure
Vs temperature derivative	km/sK	$\Delta - Vs$	High temperature
Vs recalculated at room pressure[b]	km/s	Vs_0	Recalculated at room pressure[b]
Vp and Vs anisotropy	%		Room pressure and temperature

[a] Only borehole data

[b] Calculated at 0 MPa pressure using the dV pressure derivative of experiments conducted at high confining pressure; see text for explanation

all outcropping in the Ivrea-Verbano Zone. The Ivrea-Verbano Zone is a metamorphic unit in the Southalpine domain and it provides one of the most spectacular sections through rocks of lower crustal provenance (e.g. Fountain, 1976; Pistone et al., 2017; Schmid et al., 2017; Zingg, 1990). For this reason, the data originating from the Ivrea-Verbano Zone have been included in the dbase as representatives of deep levels of a continental crust. The Ivrea-Verbano Zone is an example of an area outside the Swiss territory that was included in the dbase because of its importance in representing crustal levels that otherwise could not be adequately described. Another example of data outside the Swiss borders that were inserted in the dbase is the borehole in Humilly, in France, because they add a good sampling of crustal levels otherwise not adequately described. The 3.5 km borehole from Total (Hefny et al., 2020) crosscuts the stratigraphic sequence of the Geneva sedimentary basin (see Fig. 1). Most of the borehole was cored, and the cores, stored and made available at the rock repository of Total in the south of France, were adequate for extraction of 2.52 cm cores for experimental testing in the rock deformation laboratory at ETH. The dataset deriving from experimental tests on those cores represent a valuable petro-physical characterization of the Swiss Molasses sediments otherwise difficult to obtain from outcrop data. The data are included in the SAPHYR dbase (Hefny et al., 2020).

Nevertheless we decided to limit the data origin to regions within and in the near vicinity of Switzerland, and we did not extend our collection to all the possible crustal rock-types that are reported in literature and might be relevant for other tectonic settings or other types of continental crust.

3 Quality and uncertainty assessment

While the details of the physical rock properties collected are described in Additional file 1: S4 "dbase of physical rock properties", here we want to describe the logic flow we used to perform the quality screening of the data that went into the dbase. Furthermore, we describe the procedure we used to attribute the set of values, describing the distribution and the uncertainty of each physical property to every rock type or rock group. We want to underline that not all the rock types we considered are equally well represented and defined in terms of physical properties. Therefore, the dbase should be continuously updated in the future. In the following sections we describe the criteria we used to building up the current SAPHYR dbase and we propose that the same criteria will be used for future updates. For this purpose we outline in detail the procedure of eligibility for collection of the data, and the quality control that we applied.

3.1 Criteria of eligibility for collection and information completeness assessment

In order to be eligible for the SAPHYR collection, data had to fulfill some general quality criteria, listed below.

- Unequivocal identification: this criterion is particularly important for literature data, and aims to avoid that a single data can enter twice or more into the data base. It means that each data is linked to a sample with clear identity (sample name and its origin at least). This identification allows to attribute an ID tag to the sample in the dbase, and to link it to each physical property measured on it.
- Rock type identification: an adequate description of the rock type has to be available for each sample in order to infer the main rock forming minerals and the principal textural characteristics that can play a fundamental role on physical properties.
- Geographical identification: SAPHYR being a GIS based database, it is necessary to know the geographic coordinates of each sample to which data are linked. In the event that latitude, longitude and altitude (or depth, in case of borehole or tunnel data) were not reported in literature, or not registered for samples of already available collections, the geographic location was calculated, with the aid of maps and sample descriptions. Only if a reasonable confidence could be reached (resolution of 100 m or 10 s in latitude and longitude), the data could be used for GIS application. In the few cases where the geographic coordinates could not be retrieved the data were not inserted in the dbase.
- Experimental methodology identification: the experimental methods, conditions (pressure, temperature, fluid presence, etc.) and the error for each data. This criterion is particularly important to evaluate the homogeneity of experimental results. An example of this criterion is given by the collection of the property "density". Numerous methods can be used in the laboratory to determine density, generally together with porosity. The most common are by saturation weight and Boyle's law. However, different saturation fluids access different pore dimension, leading to different density estimations. All methods produce valid data, but they are kept separate because they refer to slightly different physical entities.

The eligibility elements stated above define a first level of information completeness, a "conditio sine qua non" for the data to be inserted in the dbase. Additional information on each data that helped us to evaluate the internal consistency of the data were considered during the process of data collection, and contribute to

the definition of the quality of the data. For example, one of the necessary requirements was the availability of the coordinates of the sampling location, together with a description of the rock type. This information is essential to allow cross-checking with independently published surface geology maps. Moreover the mineralogical composition, when available, was used to verify the rock type definition. Therefore all available complementary data were also collected as metadata. Another information that we considered as necessary, was a clear description of the method used to obtain each reported physical rock property. We collected data deriving only from standardized methodologies, in order to guarantee uniformity in each set of properties. Data collected with different methodologies were not automatically grouped and treated as uniform data. For example, porosity is measured either directly with porosimetry techniques or calculated trough densities comparisons: the sets of data were not grouped all together and used for statistical treatment, but kept as separate groups on the basis of the method used to obtain the data.

A second level of completeness that we evaluated was the areal coverage of data collection. It was based at first simply on geographical distribution and representation of tectonic units by the data. Simply superimposing the samples location available in literature on the geotechnical map of Switzerland version 1/2000 (Federal Office of Topography, 2006), we estimated the geographical distribution and sampling coverage of the main tectonic units (Fig. 1, inset). Already from a first screening it was clear that the Swiss Molasse basin sediments and their underlying Mesozoic sedimentary basement were scarcely represented in literature. Furthermore, also data from the Jura units (tabular and folded Jura) outcropping north of the Molasse basin, and data from the Flysch units outcropping south of it, were sparse. The Helvetic external units were also poorly represented (Fig. 1, inset). On the other hand, all other main Alpine units were well sampled. The acquisition of a sample collection of 261 cores from the Institute of Geophysics of ETH Zurich, where thermal properties were already measured and reported in previous studies, represented a major addition for the SAPHYR dbase. This collection represented a precious increment of data population from the Helvetic external units and added a few data points from the Jura and the Molasse. In parallel with limited sampling campaigns on outcrops of the Jura domains, the acquisition of samples from different NAGRA (https://www.nagra.ch/de/downl oadcenter.htm) boreholes located in the northeastern part of the Molasse and lately the acquisition of the borehole samples from the Geneva basin, allowed to nicely close the gaps in the original geographical distribution.

Not only geographical coverage was considered but also completeness of data population in terms of representativity of all crustal levels was also evaluated. While literature data from outcrops in the Southalpine domain, in particular in the Ivrea-Verbano zone, provided already a good coverage of the lowermost part of the crust, data from outcrops and tunnels from the Alpine chain offered good coverage over a great variety of crystalline and metamorphic lithologies of all middle crustal levels. Mesozoic and Cenozoic sedimentary sequences are represented almost exclusively by data from cores drilled in boreholes and reported on NAGRA technical reports (https://www.nagra.ch/de/cat/publikationen/technische berichte-ntbs/downloadcenter.htm).

A third level of completeness that we aimed at was to obtain on a single rock type, and when possible on a single rock sample, as much diversified properties as possible. This could be reached by new measurements campaigns on new or acquired rock samples. The main laboratories involved in the new measurements were the Rock Deformation Laboratory and the Magnetic Laboratory of the Department of Earth Sciences—ETH in Zurich. Because the 261 cores from the Institute of Geophysics of ETH Zurich were suitable in dimensions for multiple measurements, additional measurements of density, ultrasound velocities and magnetic susceptibility were obtained on the cores where thermal properties were previously measured. Very recently collaboration with the Mechanical Engineering Department of ETH Zürich allowed to expand the collection of thermal properties adding heat capacity data on few selected rock specimens.

3.2 Standard measurement procedures reported in literature

Data reported in literature and collected in the dbase were measured over a large period of time by several laboratories in Switzerland and abroad, using a variety of different techniques. All data collected fulfilled the criteria of eligibility mentioned above, i.e. they were clearly identifiable, the geographical coordinates were known or could be reconstructed from available complementary information, the methods to collect the data was clearly indicated. This section reports on and discusses only some of the most common techniques used to produce the data, being aware that an exhaustive description of all the techniques used for all the data is not possible in this study.

Grain and bulk density All rocks are always more or less porous, which is why their bulk density is always smaller than the specific weight (grain density). The bulk density value is therefore directly dependent on the mineralogical composition (grain density) and the pore space

of the sample. The determination of the bulk density together with the grain density is used to determine the absolute porosity.

The method to determine bulk density is based on weighing the sample in air and measuring the volume of specimen of regular shapes (generally cylinders or cubes) and few cm in dimensions, either with a Vernier calliper, or by buoyancy in mercury or water. The grain density (specific gravity) was generally measured with a pycnometer on rock powders or solid samples. A detailed description of the methodology adopted for most of the samples from borehole both for density and porosity is given in Müller (1964) and Peters et al. (1985), for tunnels and in outcrops in Kästner et al. (2020).

The method used for *seismic velocity* measurements for almost all the data on outcrops reported from literature is based on the pulse transmission technique described by Birch (1960, 1961). An ultrasound wave (P or S) propagates through a rock specimen mounted between piezosensors. The velocity is calculated through the time of transfer and the length of the specimen. This technique is routinely used since many decades in laboratory analyses to study elastic properties and seismic anisotropy of rocks, using either cylindrical (e.g. Kästner et al., 2020; Zappone et al., 2000), cubic (e.g. Kern, 1990) or spherical (Pros et al., 2003) specimens. Velocities from borehole samples were either measured with the Birch method (Barberini et al., 2007; Birch, 1960, 1961; Sarout et al., 2012), or with the dipole sonic imager (NAGRA NTB 00-01). The sonic probe measures the propagation of the wave trains of ultrasonic signals propagating along the borehole wall. Using different sources, the velocities of the compression and shear waves are determined.

The *permeability of rock* for liquids or gases is determined in the laboratory with permeameters using air (Müller, 1964) or helium (Pini et al., 2009) as the flowing medium. The methods are based on placing cylindrical samples between an up-stream and a down-stream reservoir, at different pressure. For methods based on constant pressure difference, the pressure in the up- and down-stream are kept constant and the flow through the sample is measured. For transient step methods (e.g. Brace et al., 1968; Pini et al., 2009) the pressure in the up and down-stream reservoirs are allowed to re-equilibrate and the permeability is measured through the time at which the two reservoirs reach equilibrium. Since permeability is a directional property, whenever possible, specimens were drilled parallel and perpendicular to the stratification or foliation.

Magnetic susceptibility is the ratio of the intensity of magnetization produced in the material over the applied magnetic field that induces the magnetization. Older methods to measure it are based on force effects of magnetic field to magnetized specimen. Inductive methods use a change of coil inductance, when the magnetically conductive specimen is embedded. Modern methods are based on magnetic resonance. Most of the data on magnetic susceptibility in the dbase were measured using inductive methods (Almqvist et al., 2010; Hirt-Tasillo, 1986).

Thermal conductivity determinations have been performed using mostly the transient line source method on dry and water-saturated samples. In these cases, a long and thin heating source (the needle probe) is inserted into a sample or placed on top of the sample surface (probe for plane surfaces) and is heated with constant power while recording the temperature rise with time inside the source. Thermal conductivity is calculated from temperature through the slope of the line for temperature rise over the log of time (Leu et al., 1999; Schärli & Rybach, 1984).

Most of the *specific heat capacity* measurements were performed by using the method of mixtures as described in Schärli and Rybach (2001). The method is based on the usage of a so-called calorimeter, a vessel of known specific heat capacity and mass, partially filled with water at a known temperature and then thermally insulated. The samples are cooled or heated either in a bath of ice and water, or in boiling water, respectively, and then quickly transferred to the calorimeter. The specific heat is then determined through the variation of temperature induced in the calorimeter.

Gamma-ray spectrometry is the most frequently used technique for determination of *heat production* (Kissling et al., 1978; Rybach et al., 1977); it enables the simultaneous determination of U, Th and K, the relevant heat-producing radioelements.

For anisotropic properties, measurements were performed, where possible, parallel and perpendicular to banding or foliation.

3.3 Standard measurement procedures for new measurements

As previously mentioned, the new measurements represent a significant contribution to the collection of densities, magnetic properties and ultrasound shear velocities. In particular, the density and ultrasound velocity (P and S) of about 350 new samples were measured in the Rock Deformation Laboratory at ETH Zurich. A big part of this new data acquisition derives from a sample collection kindly provided by Prof. L. Rybach (ETH Zurich), for which thermal properties were already measured. Of all rocks samples we knew the geographical coordinates and rock type. With this new data acquisition we aimed at a better coverage of areal distribution and an increased number of samples representative for a large variety of

rock types. Moreover, multiple properties were measured on the same samples, i.e. density, porosity, velocities, magnetic properties, and for a limited subset of samples new thermal properties were acquired. In the following paragraphs we provide an overview description of the experimental procedures used to determine those data. More and specific details may be found in the referenced literature.

3.3.1 Bulk and grain densities and porosity

The samples were cylindrical cores of 22 mm or 25.4 mm diameter and variable length of about 35 mm, dried in a 100 °C oven for at least 12 h to remove possible fluids in the pore space. Bulk density was determined as the ratio between dry mass (g) and bulk volume (cm^3), using a digital mass balance (1 mg resolution) and a digital calliper (10 μm resolution). When multiple cores from one rock sample or one locality existed, the average bulk density was considered. Uncertainty estimates for bulk density is in the order of 0.2%. Grain density was measured with the aid of a Helium pycnometer. The difference between bulk and grain density allowed the calculation of porosity. Mercury porosimetry data on porosity available in literature have been kept separate from porosity measurements obtained with this method. Similarly, density data using other buoyant methods, present in literature, have been kept separate.

3.3.2 Ultrasonic velocities (P and S)

P- and S-wave velocities (Vp, Vs) were determined using the pulse transmission technique (Birch, 1960, 1961). Experiments were performed employing either a Paterson-type gas-medium testing machine (Paterson, 1990), following technical modifications and experiment procedures described in, e.g., Faccenda et al. (2007) and Almqvist et al. (2010), or employing an oil-medium hydrostatic pressure vessel modified for ultrasonic velocity testing (e.g. Wagner et al., 1999; Zappone et al., 2000). Most of the velocities were measured at room temperature and at increasing confining pressure up to 400 MPa, (for more details of the procedure see above references). Only for few samples we had the opportunity to perform measurements at increasing temperature together with increasing pressure. The propagation error, including errors in measuring the sample length and the uncertainty in picking the first time arrival, which are the major error sources, is calculated to be around 1% for both P and S waves.

An example of Vp plotted versus confining pressure is shown in Fig. 5. A typical relatively steep non-linear increase of the velocity curve with pressure up to generally 150 MPa is followed by a linear increase of Vp at high pressure. The non-linear part of the curve is attributed to the closing of pores and cracks (e.g. Birch, 1961; Brace, 1965; Christensen, 1966; Kern & Schenk, 1985; Wepfer & Christensen, 1991), while the linear part reflects the intrinsic seismic properties of the rock, dominated by the compressibility of the crystalline skeleton. It is frequently observed that some of the void space that closes during pressurisation does not reopen during depressurisation. Therefore, velocities measured during pressurisation are typically lower than during depressurisation (e.g. Birch, 1960). The velocity hysteresis can be quite remarkable, depending on the elasticity of pores and cracks present in the cores. The reproducibility of the curve at increasing pressure is limited, therefore only seismic velocities derived during depressurisation are considered for the SAPHYR dbase. The velocity–pressure derivatives have been calculated using best-fit solutions from the linear part of the velocity–pressure relation. The velocities at room pressure (nominally 0 MPa) have been obtained by linear extrapolation, using the pressure derivatives (Fig. 5).
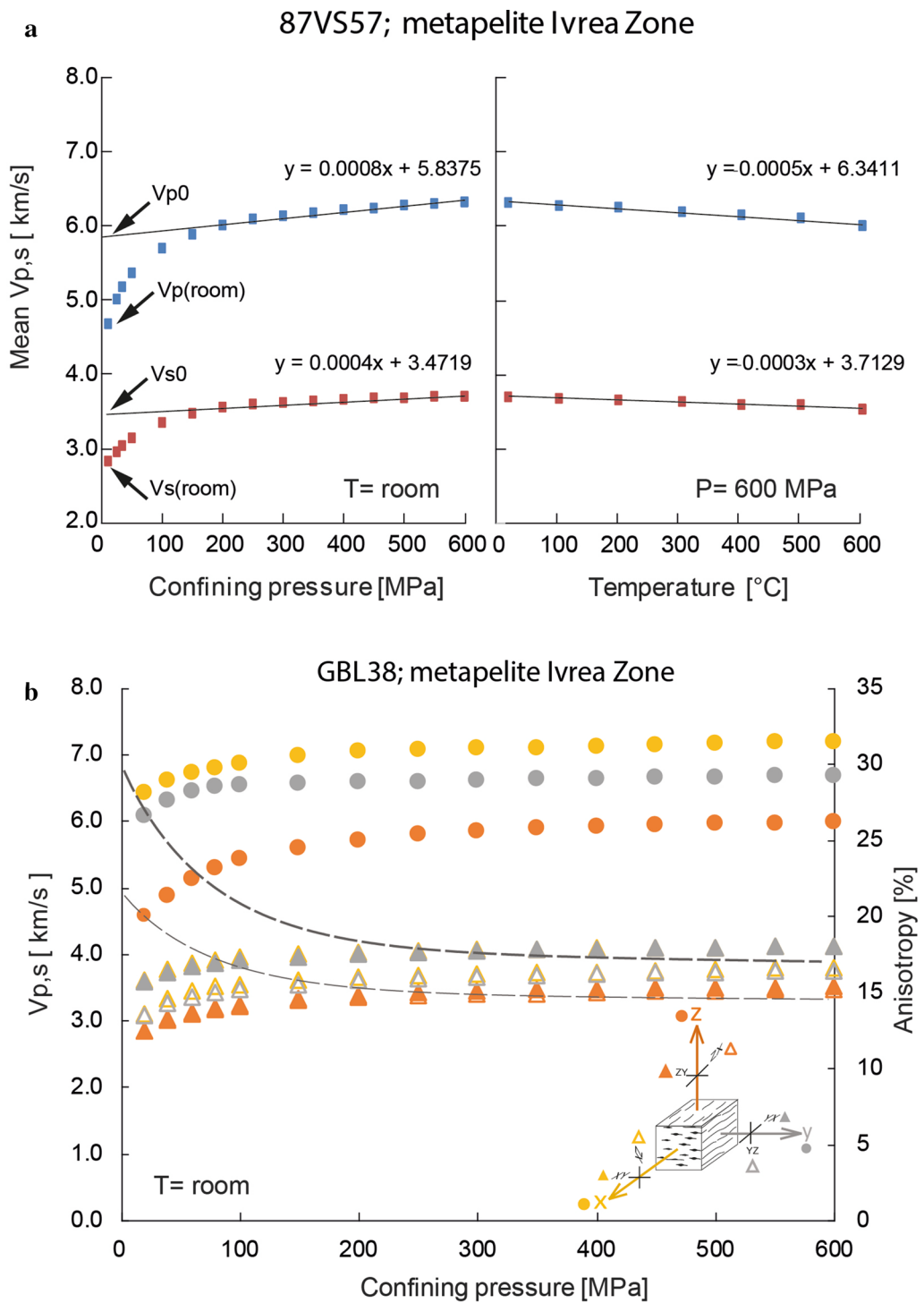
To determine the directional dependence of the seismic wave velocities, where the sample dimension made it possible, three mutually perpendicular cores were drilled parallel to the rock fabric (foliation and lineation in crystalline rocks, sedimentary plane in sedimentary rocks). The convention used to name the cores is visualised in the inset of Fig. 5: X is the direction parallel to mineral lineation, Y is normal to the lineation and Z is normal to the foliation. While for some purposes a bulk velocity value might be sufficient, for many applications this dependency is important (Fig. 5). Values for Vp0, Vs0 are derived in the three directions, and the respective pressure derivatives were included in the SAPHYR dbase. Moreover, anisotropy and the average values of the three directions have been collected in the SAPHYR dbase. Unfortunately up to now S-wave measurements are far fewer in numbers than P-waves.

3.3.3 Magnetic properties

All new magnetic data were performed at the Laboratory of Natural Magnetism, ETH Zurich. Magnetic measurements include determination of susceptibility and anisotropy of susceptibility (AMS) acquisition. The measurements were performed on an Agico (Brno, Czech Republic) KLY2 susceptibility bridge (see Jelínek & Pokorný, 1997 for technical details). For AMS, we measured 15 directions to calculate the ellipsoid/full susceptibility tensor and computed the mean susceptibility from that.

3.3.4 Thermal properties

Thermal properties were all taken from literature data, either from scientific publications or from public and

a 87VS57; metapelite Ivrea Zone

(P-plot, T= room) $y = 0.0008x + 5.8375$ (Vp0, Vp(room)); $y = 0.0004x + 3.4719$ (Vs0, Vs(room))

(T-plot, P= 600 MPa) $y = 0.0005x + 6.3411$; $y = 0.0003x + 3.7129$

Mean Vp,s [km/s] vs Confining pressure [MPa] / Temperature [°C]

b GBL38; metapelite Ivrea Zone

Vp,s [km/s] vs Confining pressure [MPa]; Anisotropy [%]; T= room

Fig. 5 Example of velocity curves from laboratory experiments (error bars within the symbols). **a**, **b** Effect of increasing pressure and temperature respectively on P and S waves; In **a** it is shown how intrinsic Vp0 and Vs0 calculated from the intercept of the linear regression of the high pressure part of the curve (here above 150 MPa), and how they differ from room pressure. While for some application a "bulk" velocity might be sufficient, for many other applications the dependency of velocity over the direction of measurement and the anisotropy are important. **c** Shows a complete dataset of velocities measured along the main structural direction X = parallel to lineation, Y = perpendicular to lineation in the foliation or bedding plane, and Z perpendicular to foliation or bedding, as shown in the inset. Vs measured along the three structural direction are distinguished on the basis of the polarization plane, as shown in the inset. As Example Vszy is the S waves propagating perpendicular to foliation and with polarization in the zy plane, i.e. the plane normal to lineation. In this example, the velocities measured along the structural directions are quite different. The anisotropy calculated as (Vmax − Vmin)/V average is also show in think dash line for Vp, and in grey dash line for Vs

semi-public reports. The data were mainly obtained by the former Thermal Properties Laboratory at the Institute of Geophysics ETH Zurich (e.g. Rybach & Pfister, 1994; Schärli & Rybach, 2001) and more recently from a private laboratory with rigs working under the same experimental conditions. Very recently, thanks to a collaboration with the Engineering Department at ETH new data on specific heat capacity have been collected and introduced in the dbase (Becattini et al., 2017). The specific heat capacity was measured with the aid of a Setaram DSC 121 heat flux calorimeter for routine determination of the heat capacity of solids above ambient temperature. The heat capacity is measured by comparing the amount of heat required to increase temperature in the sample and in a standard rock of known heat capacity. The measurements could be performed up to 1000 °C. The main limitation of the apparatus is in the dimension of the samples, a few mm, which limit its application to very fine grained rocks.

4 Results

4.1 Definition of lithological groups

Based on the information that could be retrieved about the specimens (rock type, mineralogical composition, modal composition, textural description, etc.) we classified the samples in broad rock types, following the classical criteria of classification for sedimentary, igneous and metamorphic rocks (e.g. Charmichael, 1989; Carmichael & Klein, 2020). We adopted the classical petrological (e.g. Jahns & Kudo, 2020) and sedimentological (e.g. Bissell et al., 2020) terminology, commonly in use in geological literature, but we preferred always terms describing the mineralogical composition and microstructure rather than the petrogenesis. For example we preferred the terms "feldspar gneiss", "mica-bearing gneiss" and "schists" to the terms orthogneiss and paragneiss, because many physical properties are mainly related to mineral and modal composition and rock texture. We defined in this way 26 rock types (see Additional file 1: S2 "lithology list") for which we had obtained a sufficient number of physical properties.

Subsequently, we grouped the 26 rock types in 22 lithological groups, establishing a correlation between each lithological group and the 69 lithology types that are listed in the legend of the geotechnical map of Switzerland (Federal Office of Topography, 2006) version 1/2000, map scale of 1:500,000, as shown in Additional file 1: S2 "lithology list". This correlation was necessary in order to represent the distribution of physical properties with statistical significance (namely density and velocity) on a map. Water, ice, unconsolidated debris and unconsolidated fine-grained deposits are also listed in the table for completeness, but no data were collected for them

and the values that were used to compile the maps (see Sect. 5) were taken from literature and refer to worldwide data.

While for the majority of rock types the classification in a lithological group has been straightforward, in some cases the attribution to a specific lithological group has been less certain and somehow subjective. This difficulty arises because in SAPHYR we are interested in lithologies that are representative of the whole continental crust (including its deepest parts) with regard to physical properties of rocks, while in the geotechnical map (Federal Office of Topography, 2006) the legend is designed to represent the technical use of the shallow subsurface (extraction of mineral resources, building projects) and the rocks are subdivided according to their formation (genesis).

In order to explain the compromising efforts we quote, f.e., the case of conglomerates and breccias. The two lithotypes are jointly mapped in the geotechnical map (Federal Office of Topography, 2006), but the two terms in a broad sense refer to rocks of different origin: conglomerate is a coarse-grained clastic sedimentary rock that is composed of a substantial fraction of rounded to sub-angular gravel-size clasts; breccia is a rock composed of broken fragments of minerals or rock cemented together by a fine-grained matrix and it may derive from igneous or sedimentary rocks (e.g. Shukla & Sharm, 2018). As a result of the different origins and consequently different mineral and textural composition, the physical properties of the breccias and conglomerates are statistically quite different (see the example of density in Fig. 6a) with breccias showing a density range twice as large as that of conglomerates. Thus for our purposes it makes sense to keep the two rock types separate in the dbase. The treatment of this and analog cases in the map preparation phase is explained later in the text.

Another example of a case where the lithology classification we adopted was more detailed that in the geotechnical map (Federal Office of Topography, 2006) is the case of tonalities and granodiorites. Both rock types are relatively abundant in the laboratory data from literature, but not frequently enough encountered in surface outcrops to be mapped separately at the scale of the geotechnical map (Federal Office of Topography, 2006) and, therefore, neglected in its legend. We kept tonalites and granodiorites as separate groups in the dbase even if it is impossible to distinguish their outcrops on the maps. The same case applies to rock types typical of lower crust in the Ivrea-Verbano Zone such as kingizites, stronalites (Bertolani & Garuti, 1970), granulites, that are quite important for the representation and modeling of the lowermost part of the continental crust (see Fig. 6b).
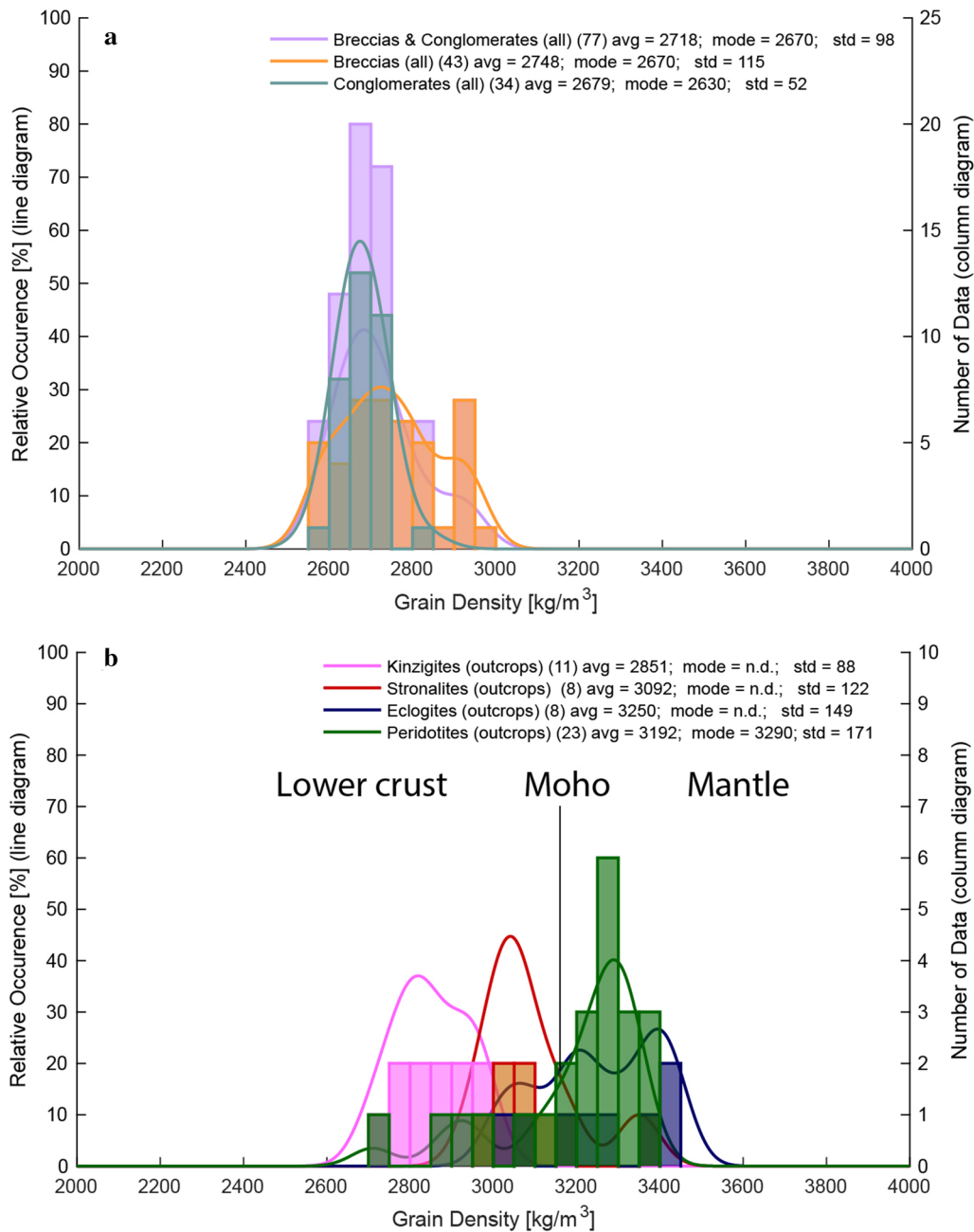
Fig. 6 Examples of density distributions for **a** breccias and conglomerates and **b** for lower crustal (kinzigites, stronalites) and uppermost mantle (peridotites, eclogites) lithologies, separated by the crust-mantle boundary (Moho). The diagrams show a visual comparison of block histograms and respective kernel distributions (solid lines) generated from the density data. Histograms refer to the number of data (on the right vertical axis) falling in a specific densities range, here in steps of 50 kg/cm^3. The numbers in parenthesis represent the total number of data for each distribution. For example, in the case of breccias, 10 of 45 samples available have densities in the range 2900–2950 kg/cm^3. Solid curves represent the Kernel smoothing function calculated over the density data population and representing the relative occurrence of density values in % (left axis). The Kernel distribution builds a function to represent the probability distribution of the sample data. **a** The density distributions for conglomerates and breccias (from boreholes and outcrops combined) document a much wider range of values for breccias that, when combined in one single lithology group would indicate two maxima. The mode is also indicated, but not in all cases it could be calculated (n.d = not determined). **b** Density values for rock types from the Ivrea-Verbano zone. The density distributions of the Kinzigites, Stronalites and Peridotites/Eclogites exhibit three distinctively different maxima reflecting the different mineral and modal composition and documenting the difference in density across the Moho discontinuity between the lowermost crust and the mantle lithosphere

In most of the cases, however, it was not necessary to add details and subdivisions to the lithology list of the geotechnical map (Federal Office of Topography, 2006). On the contrary, more often it was necessary to group geotechnical-lithological units into broader rock types units. A good example is the case of sandstones, the composition of which may vary over a broad range, depending on the nature and amount of the cementing matrix, on the grain size and the sorting, on the degree of compaction and therefore on the porosity, or on the interlayering with other sediments. Such a fine distinction (interlayering, compaction) is beyond our knowledge from the single laboratory sample, or too arbitrary to be applied systematically to the whole data population. Therefore, we used the term "sandstone" in its broader sense, with the consequence that many physical properties measured at outcrop conditions are distributed over a wide range of values.

In terms of representativeness and for visualization of physical properties on GIS maps, an advantage to group the original lithology types of the geotechnical map (Federal Office of Topography, 2006) into general lithology groups (in total 20 groups referring to solid rocks and three more to unconsolidated deposits, ice and water) is the increase of data population for each lithology available. Once our data were grouped in rock types, it was straightforward to identify the rock types of which we did not have a sufficient number of samples (a minimum value of 7 for each rock type was arbitrarily chosen) in order to perform statistical analysis (as described in Sect. 2), and for which new sampling and measurements was needed, as described in Sect. 3.3.

4.2 The multi-layered tabular dbase

The available data have been collected and organized in Microsoft Excel spread sheets where each sample is identified through its name and geographic coordinates. We choose the form of spread-sheets because it provides the easiest way to import them directly into ArcGIS (ESRI 2011. ArcGIS Desktop: Release 10. Redlands, CA: Environmental Systems Research Institute), the selected geographic information system (GIS) for working with maps and geographic information in this study. ArcGIS was then used for creating maps of the areal distribution of the physical properties, as explained later in Sect. 5 dedicated to maps description. To localize the samples, we adopted the Swiss geographic coordinate system, therefore all latitudes and longitudes have been recalculated in Cartesian coordinates. Altitude, or depth in case of borehole or tunnel data is also recorded.

We kept two separate dbase parts, one for boreholes and one for outcrops. The dbase on boreholes refers to data reported by NAGRA reports and regards deep boreholes (more than 1 km depth) in the Swiss plateau. The dbase referring to outcrop data also contains data from tunnels and shallow boreholes that are identified by a special code. As borehole samples are collected at different depth, their physical properties (or at least part of them) might be influenced by the burial history, and equally the properties collected from outcrop samples might be affected by the exhumation history.

In the same spread-sheets we assembled information about rock type, geologic unit or stratigraphic unit, and tectonic unit, together with all the physical properties measured on the sample and their respective error estimates, when available. The source of the information (literature reference, public or private report, unpublished data with laboratory and authors' names) was also recorded for each data. No data of unknown origin was inserted in the dbase.

In the dbase, data have been grouped on the basis of the physical property and on the basis of the measurements procedure. Error estimates for each properties were recorded as well, when present in the original documents, or calculated for new measurements. When necessary, data were recalculated in SI units.

4.3 Physical property processing

Each data collected in the spread-sheets represent a local point source of information. The aim of the dbase is not only to collect in a systematic way the physical properties available from laboratory experiments, but to also present them in the perspective of the assembled data of same kind (physical property) from same lithology to provide the user of the dbase with information about the representativeness of the individual data and finally to display the data on bulk density or ultrasound velocity as thematic maps.

The primary goals of the processing are to identify the range and distribution of the values and their uncertainties for every physical property and every lithology. To establish those distributions and to obtain uncertainties we take into account the reliability and uncertainty of the individual data and, in particular, search for and identify outliers that result from wrong information.

By analyzing the distributions with a statistically significant number of data for each property and rock type, it was possible to identify several cases with mistaken reports of lithology, location or obviously erroneous measurement reports. In some cases of wrong lithology association, f.e., due to local naming, outliers in more than one property could be cross-linked and thus the data could be corrected. In all other cases, the outlier data was marked in the dbase as problematic, neglected for further processing and not used for statistical treatment for the preparation of thematic maps. The density

values were of particular usage to detect "outlier data" for reasons of wrong lithology association as these data were clearly falling outside the reasonable tails of Gaussian distributions.

4.4 Variation in density and Vp within a lithology

There is a large variability in the number of data among different physical properties and among different lithologies. When observing the number of data for each measured property as shown in Fig. 4, it is evident that the dbase contains a large amount of data for density while data for other properties such as, for example, ultrasound velocity and especially shear waves velocity data, are rare.

Density is the most often measured physical property and consequently it is the most abundant property in the dbase. Moreover, density is a simple scalar quantity and as such it does not contain the complications linked with tensor properties, namely the directionality of the measurement. For these reasons, density was used first to develop the statistical treatment of the data. The grain and bulk density data of each lithology group were used to calculate mean, median, and range distribution. When possible, the most frequently occurring, or repetitive,

value in each sample of data, the mode, was calculated too.

The physical property distribution diagrams for each lithology are provided in Additional file 1: S5 "distribution of physical properties for each lithology". Here we discuss only a few selected examples with the intent to illustrate some key observations and conclusions that can be taken from such diagrams.

Case 1   Granites—the ideal case.

Grain densities for granites are a good example of a high-quality data set. Figure 7 shows the data distribution of samples from outcrops (68 data) and boreholes (113 data). Both data sets show a narrow distribution (standard deviation of 48 kg/m^3) almost symmetric around the mean value (2640 kg/m^3 for boreholes, 2670 kg/m^3 for outcrops). The definition of granite is well constrained in the geological terminology. It refers to a specific chemistry and mineralogy and the rock for its nature is almost non-porous and exhibits no or very minor anisotropy. Moreover, the data collection is abundant, which makes the statistic treatment more solid and representative. The
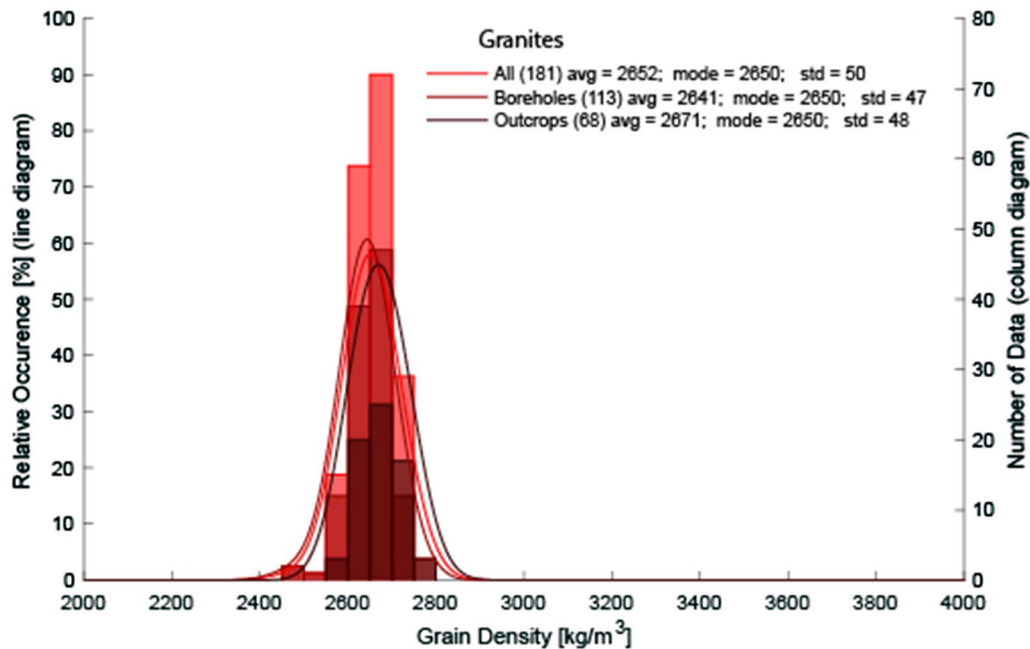
Fig. 7 Measured density values distribution for granites. The data distribution of grain density has been a valid instrument to determine and validate the criteria we adopted in grouping. The displayed distributions clearly justify merging the surface data with data at depth (borehole) for this lithology group. Numbers in parenthesis represent the total number of data. The figure provides a visual comparison of a histogram and a kernel distribution generated from the density data for granites from boreholes, outcrops and all together. Histograms refer to the number of data (on the right vertical axis) falling in a specific densities range, here in steps of 50 g/cm^3. For example, in the case of granites from boreholes, out of 113 density data available, 47 fall in the range from 2650 to 2700 g/cm^3. Solid curves represent the kernel smoothing function calculated over the density data population and representing the relative occurrence of density values in % (left axis). In granites from boreholes the value of density with max probability (here 60%) is 2641 kg/m^3

distributions of outcrops and boreholes data are quite similar, both for the reasons mentioned above and for the equally large number of data. In the case of granites, the average value of 2652 kg/m^3 with a standard deviation of 50 kg/m^3 was adopted to represent all outcrops of the units n. 50 and 51 of the geotechnical map (Federal Office of Topography, 2006) (see Sect. 5). Note further, that this value corresponds very well with the average bulk density of 2670 kg/m^3 used in standard Bouguer gravity correction for the near-surface crystalline basement rocks.

Case 2 Dolomites—boreholes versus outcrops data quality.

The case of dolomites (Fig. 8) is a good example of different data quality in outcrops and borehole data. While we have quite a large number of bulk density data from boreholes (117) only a limited number of density data derive from outcrop samples (17). As a result the distribution of outcrops data is a bit scattered, but the average values are quite similar. Nevertheless, standard deviations are in both cases relatively small, probably resulting from a relatively precise definition of the term dolomite that refers to a compact sedimentary carbonate rock that contains a high percentage of the mineral dolomite. Combining outcrop and borehole data, we obtain

an average value of 2797 g/cm^3 with a standard deviation of 76 g/cm^3 (for 134 samples) and these values were adopted as representative for the geotechnical units n. 47, 48, 49 of the geotechnical map (Federal Office of Topography, 2006).

Case 3 Ultramafic rocks—alteration and weathering.

Grain density distributions for peridotites and serpentinites present two clearly separated peaks (averages are 3192 and 2733, respectively) with a quite extended overlap area (Fig. 9) between them. The data has been confirmed by quality screening to be reliable and precise. Serpentinites are the alteration product of peridotites. Peridotites gradually transform into serpentinites due to more or less alteration of olivine (single crystal end members mineral density of 3270 kg/m^3 for fosterite up to 4390 kg/m^3 for fayalite; Chen et al., 2002) into serpentine polymorphs (mineral density of 2520–2650 kg/m^3, e.g. Deer et al., 2013, and references herein), while the excess Fe goes into magnetite. The overlapping area between the two peaks is the result of this gradual transition from pure peridotite to serpentinite. Almost all outcropping peridotites are affected by variable degree of serpentinizaiton, because the process of exhumation implies decompression and fracturing and quite often

Fig. 8 Density values distribution for dolomites. Number in parenthesis represent the total number of data. See Fig. 6 for explanation of curves and histograms. In this case, the graphs justify our choice to merge the surface data with data at depth (boreholes). The mode for outcrops and borehole data though is quite different. The difference between mode and average in the outcrop data is also significant, indicating a large uncertainty, linked to the low number of data available (18). Averages are in both cases coincident. The total data population has been used to attribute a density value of 2796 kg/m^3 and a standard deviation of 58 kg/m^3 for the dolomites

Fig. 9 Density values distributions for peridotites and serpentinites (see Fig. 7 caption for explanations). For these rock types only outcrop data were available and only in limited numbers. Both peridotites and serpentinites show distinct peaks in their distributions. The large standard deviation corresponds with the nature of the two rock types, serpentinites being the product of alteration of peridotites rather than to data variations due to measurement differences or uncertainties (see text)

fluid circulation is involved. Even a tiny amount of serpentine reduces drastically the density of the rock and affect many other physical properties, such as magnetic and seismic properties (e.g. Christensen, 1966; Fujii et al., 2016; Horen et al., 1996; Kern & Tubia, 1993; Toft et al., 1990). Therefore we believe the samples with density below 3.1 kg/m are serpentinites with relicts of peridotites. We choose the value of 3.1 as threshold on the basis of the density of olivine. It has to be noted that serpentine is stable also at great depth (Ulmer & Tromsdorff, 1995) therefore serpentinized peridotites are not only a characteristic of outcrops, but they can also be found at depth, therefore we think it is important to show also the values of "mixed" peridotites and serpentinites.

Serpentines and peridotites show quite pronounced maxima in their distribution curves that allow the attribution of two quite distinct values of density: 3193 kg/m^3 and 2726 kg/m^3 for peridotites and serpentinites, respectively. Standard deviations in both cases are quite large reflecting the above mentioned effect of progressive alteration and change in modal composition.

Case 4 Breccias and conglomerates—subdivision not representable in the geotechnical map (Federal Office of Topography, 2006).

As already mentioned, in most of the cases it was necessary to group individual lithology types of the geotectonic map into broader lithological groups (see Additional file 1: S2 "lithology list"). Only in few cases and for specific reasons we created subdivisions within the lithological types. One such example is given by breccias and conglomerates that are joined in one lithological unit in the geotectonic map (23: breccia and conglomerate, 46: calcareous breccia or conglomerate; 64: sericite-rich conglomerate and breccia) but they represent rocks of different origin. Especially a breccia may have a variety of rocks of different origins, including sedimentary breccia, tectonic breccia, igneous breccia, and impact breccia. The various origin of the breccias is reflected in a density distribution that is significantly wider compared to that of conglomerates (Fig. 6a). Nevertheless, for sedimentary breccias the difference with conglomerates is only in the shape of the clasts (more rounded in conglomerates and angular in breccias) deriving from a less mature sediment in the case of breccias. In this case the two terms largely overlap, as may be seen with the two density distributions. We decided to keep breccias separate from conglomerates in the dbase, but to adopt a common average and a large standard deviation for representation in the GIS maps.

4.5 Data presentation

The data distribution has been a valid instrument to identify outlier data and to determine and validate the criteria we adopted in the grouping of lithologies (see Additional file 1: S2 "lithology list"). For each lithology group the standard deviation was calculated assuming a Gaussian distribution around the mean value. Arbitrarily we choose a minimum number of 7 data over which to perform statistics. In other words, rock types with less than 7 measurements from different samples, f.e., of bulk density were not considered for statistical treatment and no average and standard deviation is listed in the dbase. This statistical treatment of the data for each group of rock types and of each physical property was primarily used for the assessment of the individual data quality and completeness (Sect. 4.2) and for the assessment of physical property value range, distribution and uncertainty. Subsequently, it provided also the basis to transform the data point collection into a representation of maps of physical property distribution.

The use of a GIS allows also an easy visualization of complementary data as in the examples shown in Fig. 10 for all properties measured in a sample from an outcrop (inset a) or from a borehole sample (inset b).

By recording coordinates and depth, in case of boreholes, it is easy to show from the same geographical locations many data collected on different lithologies at various depth.

Statistical information for each lithology group are presented for selected physical properties in the tables in Additional file 1: S4 "dbase of physical rock properties" and in diagram format in Additional file 1: S5 "distribution of physical properties for each lithology". Statistical data include number of available data (population size), minimum, median and maximum values, standard deviation (σ) and standard deviation interval (σ-interval). Moreover, a somewhat subjective description of the binned data distribution may provide some information about the general quality and reliability of the data.

The great amount of density data collected both from literature and by new measurements allowed the attribution of average values to the rock formations and the drawing of a surface rock density distribution map of Switzerland (Fig. 11). In parallel and in analogy with the density map, we developed a surface P-wave velocity distribution map (Fig. 12). We did not produce an analogous map for S-wave velocity because the data in
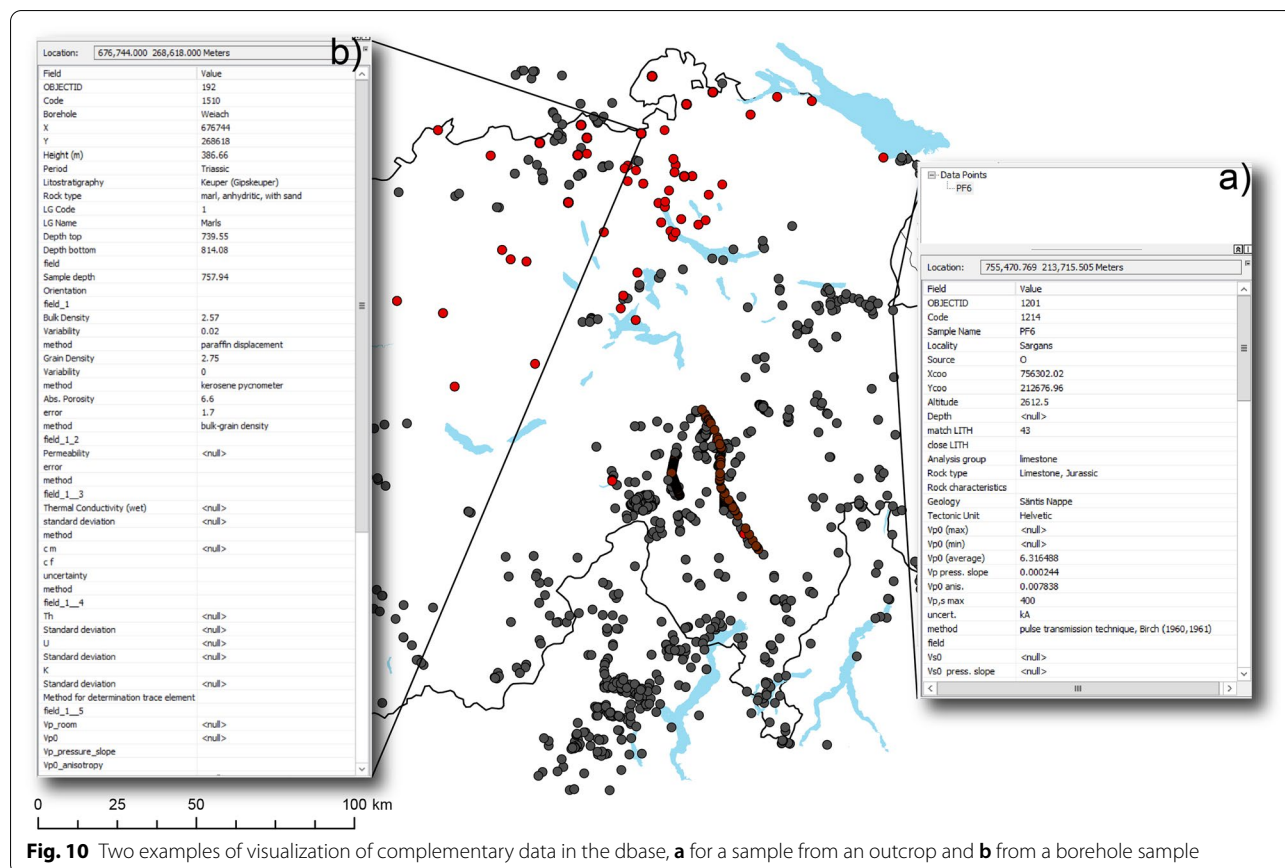
Fig. 10 Two examples of visualization of complementary data in the dbase, **a** for a sample from an outcrop and **b** from a borehole sample

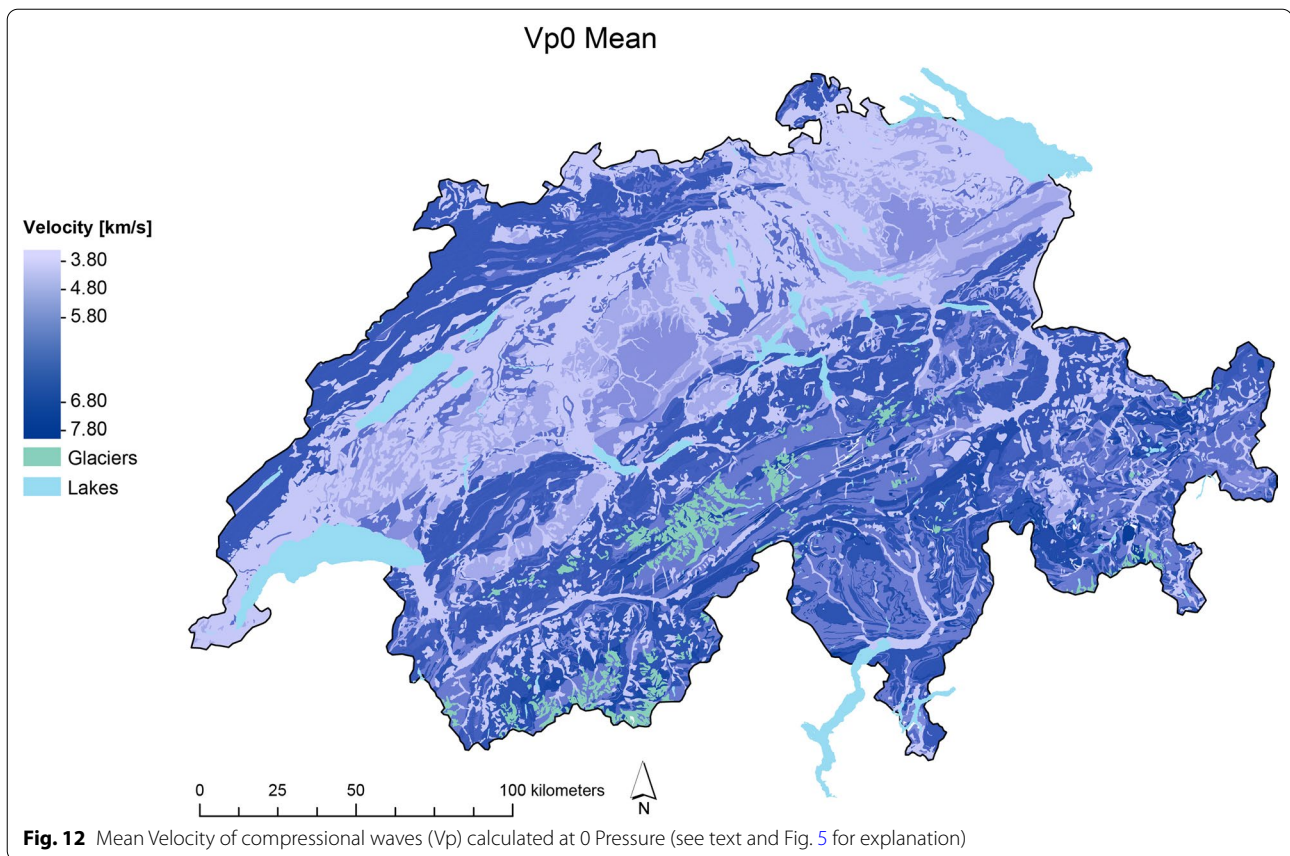**Fig. 11** Mean bulk density distribution in surface rocks of Switzerland
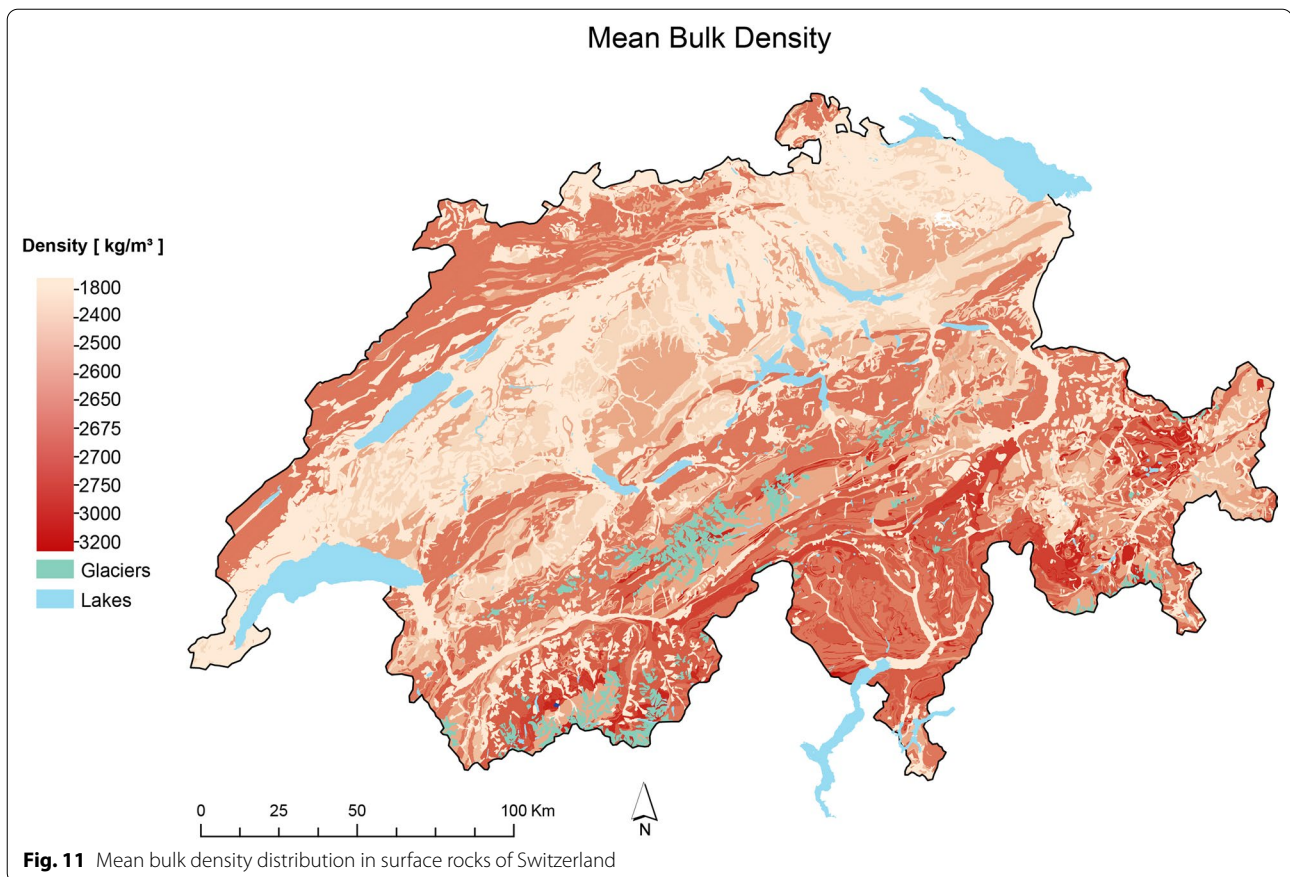
literature for S waves are scarce and the sampling does not allow a reliable extrapolation from single sample data to whole rock formation.

The tables in Additional file 1: S4 "dbase of physical rock properties" contain the individual values that were used to prepare the maps in Figs. 11 and 12. Note that data of some lithology groups (e.g. evaporites, stronalites and kinzigites) that mainly outcrop outside Switzerland do not appear in Figs. 11 and 12. Since rocks are defined as agglomerations of minerals, and minerals are naturally occurring crystals, ice as a naturally occurring crystalline substance has been considered as a rock (lithology group 21 in geotechnical map). As laboratory data for ice collected in the Swiss Alps was not available, the data reported in tables and figures have been exceptionally collected solely from worldwide literature. With reference to the dependence of ice density and velocity on temperature, only data collected in the range of $-40\,°C$ to $0\,°C$ have been considered, representing Swiss Alps temperature conditions. Unconsolidated sediments (e.g. sand, gravel, pebbles, stones and debris blocks), that are abundant at the surface, and therefore appear in many areas on

the geotechnical map (Federal Office of Topography, 2006), have been considered also as a "lithology group" and again due to lack of lab measurements density data was collected from literature reporting in situ measurements collected mainly in Switzerland (Anselmetti et al., 2010) but also worldwide (Mavko et al., 2009 and references herein; Schön, 2015 and references herein).

Figures 11 and 12 display the surface distribution of average values per lithology group of bulk rock density and P-wave velocity at surface conditions, respectively, over the entire Swiss territory. In Fig. 13 we also display the standard deviation of density for different lithological groups. Note that the standard deviation in this case does not refer to uncertainty estimates but rather it indicates the range of variability of density for each lithology group that may result from various conditions and the evolution of the rock (see, f.e., Fig. 9 and explanations in text). The effect on density from compaction by overlying mass is greatest for unconsolidated sediments as, f.e., those in the overdeepend Alpine valleys (Kissling & Schwendener, 1990) and hence, these lithology groups show the largest standard deviation (Fig. 13).

Fig. 12 Mean Velocity of compressional waves (Vp) calculated at 0 Pressure (see text and Fig. 5 for explanation)
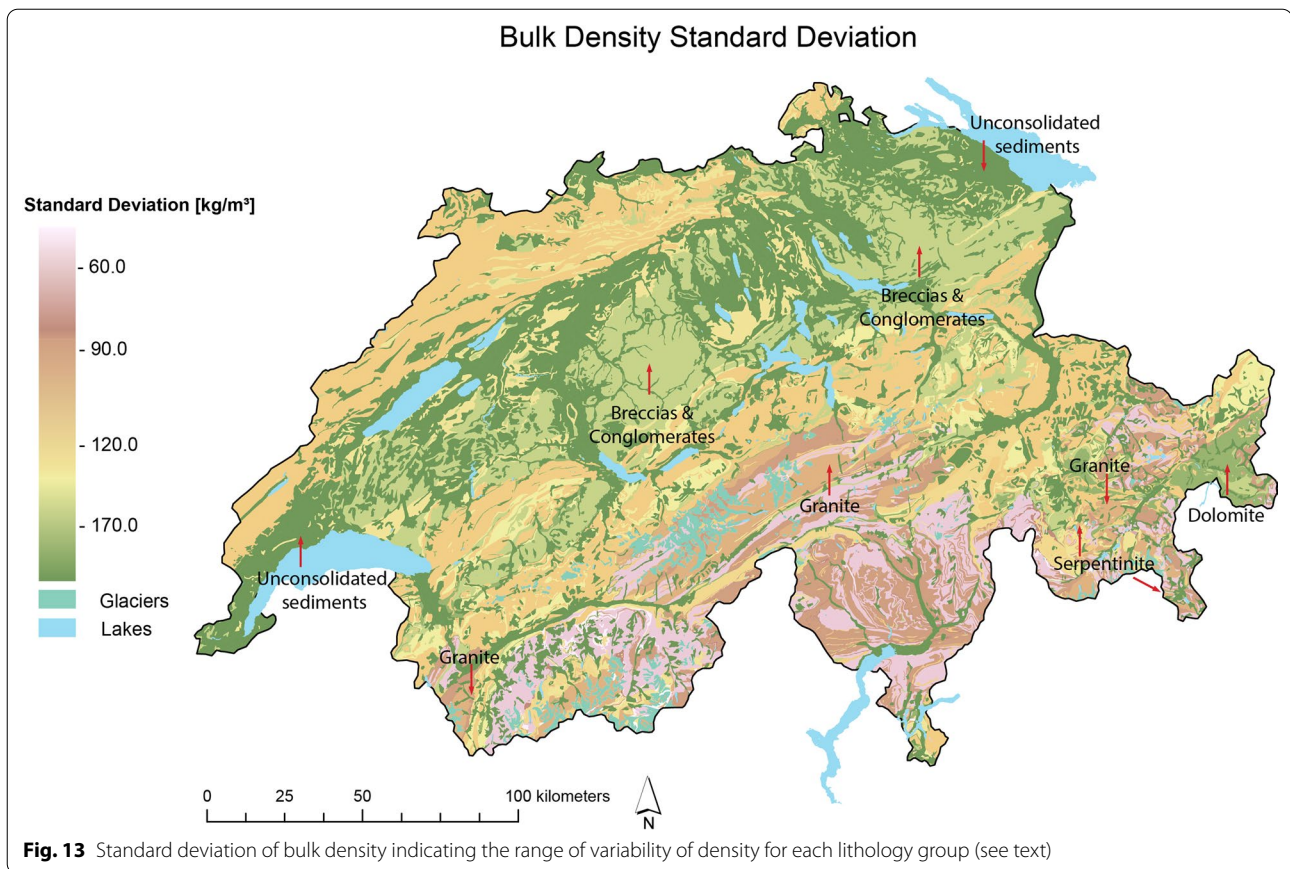
5 Discussion

The dbase contains at present more than 4500 data points, each of them representing a sample from which a single property or, in the vast majority, multiple physical properties have been measured. Nevertheless, the dbase can and will be largely improved with new data acquisition either from new literature or from new measurements.

Due to easy access and excellent outcrop conditions, the vast majority of samples originate from the Alps in southern Switzerland and northern Italy (Fig. 1). In comparison with the Alps, sampling in the Jura and Swiss central plateau (Mittelland) remains sparse (Fig. 1). A great improvement has been the inclusion in the dbase of deep borehole data that were drilled through the sedimentary sequence of the Swiss sedimentary basin down to the crystalline basement. Some lithology groups, however, still would benefit from new measurement campaigns. Moreover, even if in most cases it was documented that compaction and lithostatic pressure have no effect on many properties (e.g. grain density, heat production) in other cases the data collected from outcrops differ from the borehole data, because of the exhumation history of the surface samples (see for example of bulk density

in the limestones (in Additional file 1). Of course these observations are possible only if a large and comparable number of data from boreholes and outcrop data is available. At present only bulk and grain density have been collected to such an extent to allow these considerations.

Specific considerations on the variation of density, P-wave velocity, and a few other properties have been elaborated in this study for several lithologies with significant number of observations and the spatial distribution within Switzerland of average bulk density and P-wave velocity have been presented for all lithologies. In many cases though the dbase currently is too small to reliably derive from individual measurements representative values for specific lithologies and physical properties as it should be expected that a more abundant number of data might change quite substantially the data distribution.

Nevertheless, the currently available dbase allows a few examples of more general observations and interpretations. A general observation is that in almost all the distribution of bulk densities the distribution is slightly asymmetric with a tendency to an elongated side or tail towards low values (negative skew). This is partly due to the process of identifying outliers: while data falling completely out of the normal distribution

Fig. 13 Standard deviation of bulk density indicating the range of variability of density for each lithology group (see text)
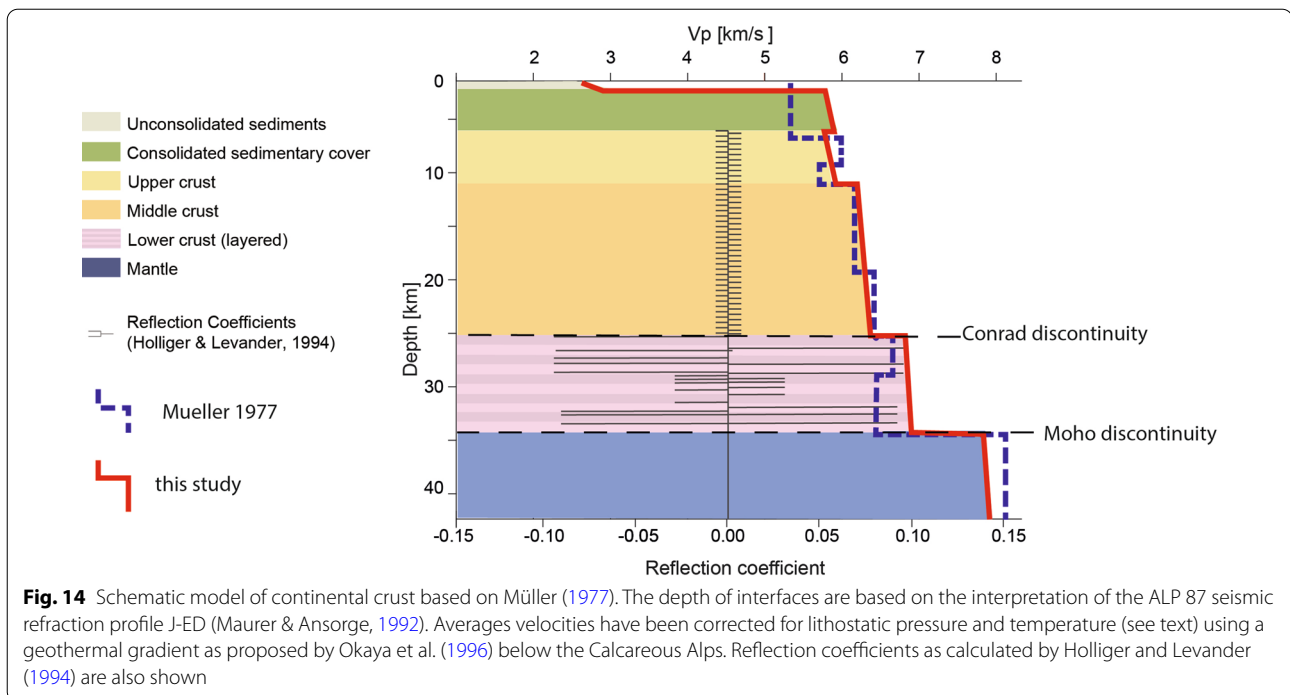
because of very high values can be considered outliers, data identified with very low values cannot be excluded a priori because the value might be linked to a high porosity of the sample. In fact, the negative skew is more pronounced in sediments than in crystalline rocks though alteration of such samples, e.g. sericitization of granites or serpentinization of peridotites (Fig. 9) can also produce the negative skew. The effect of positive skew observed in gabbros possibly can be due to the mixture of magmatic gabbro, granulitic gabbros and mafic granulites in the data population. Quite often we did not have the necessary information (chemical analysis and microstructural description) to allow a distinction among the three rock types that are all in any case an aggregate of pyroxene, and calcium-plagioclase. Garnet, which in the metamorphic cases can be quite abundant (being the metamorphic product of Al rich components) would have the effect of increasing both ultrasound velocity and density. The same consideration can be done for the positive skew of marbles that may contain Ca- or Mg-silicates and Al-silicates in variable amounts, as metamorphic products of limestones containing silica or dolomite. Only in some cases where we had detailed information on the mineralogical

composition we could prove that the high values could be linked to these mineral components.

All bulk density data (1904) show a density distribution between 1860 and 3429 kg/m^3, with a standard deviation of 228 kg/m^3 and a mean of 2628 kg/m^3, which is a value close to the average density for surface topography corrections assumed in gravity models (e.g. 2670 kg/m^3, Hinze, 2003). It must be noted, however, that this value represents just the average density of the uppermost continental crust (possibly top 5 km, Christensen & Mooney, 1995) and a notable increase in bulk density is expected and sometimes observed due to increasing lithostatic pressure and temperature and, in particular, due to systematic variation in mineralogy with depth (see below). Derivatives with pressure and (fewer) with temperature are in any case available in the dbase and would allow for these correction, if requested for detailed studies.

By separating lithological groups into sedimentary and igneous upper crustal rocks (LG 2, 3, 4, 5, 7, 13, 8, 11), mid-grade metamorphic and silicic intrusive middle crustal rocks (LG 6, 9, 12, 14, 15, 16, 17, 24) and lower crustal high-grade metamorphic mafic and ultramafic rocks (LG 10, 19, 20, 24 and 25) it is possible to establish a continental crustal model (Fig. 14) along the proposed

Fig. 14 Schematic model of continental crust based on Müller (1977). The depth of interfaces are based on the interpretation of the ALP 87 seismic refraction profile J-ED (Maurer & Ansorge, 1992). Averages velocities have been corrected for lithostatic pressure and temperature (see text) using a geothermal gradient as proposed by Okaya et al. (1996) below the Calcareous Alps. Reflection coefficients as calculated by Holliger and Levander (1994) are also shown

model of Müller (1977) for central Europe and to weight the contribution of the various components. With this subdivision a mean bulk density value of 2578 kg/m³ (standard deviation of the means = 64) for the upper crust, 2747 kg/m³ (standard deviation = 116) for the middle crust, and 2976 kg/m³ (standard deviation = 197) for the lower crust/upper-mantle can be assigned. When applied to a crustal model with 12% of upper crust, 38% of middle crust and 50% of lower crust, as proposed by Christensen and Mooney (1995), an average crustal density of 2841 kg/m³, can be calculated surprisingly similar (mean bulk density 2835 kg/m³) to the average that Christensen and Mooney (1995) get by using an inversion from velocity data observation worldwide. This value agrees with the density modeling for the Central and Southern Alps by Holliger and Kissling (1992), after correcting for the effects of large Molasse and Po plain sedimentary basins.

However, caution is needed in giving significance on these averages—particularly for the upper crust—because the densities of sedimentary rocks generally increase with age due to the lithification and decrease in porosity. Even in this case the dbase can provide a good tool for establishing correlation with sedimentary ages, indicating an average value of Permo-Carboniferous sedimentary rocks, that in the Swiss sedimentary basin is represented by sandstones to conglomerates, of 2425–2462 kg/cm³, while for Mesozoic sediments (mainly represented in the dbase by limestones, dolomites and claystones) the average is 2541–2561 kg/cm³ and for Cenozoic sediments (porous sandstones of the Swiss Molasse) it is 2286 kg/cm³.

Analog to averaging bulk densities for crustal layers it is possible to average measured velocities and to develop a calibrated model of P waves in the Swiss continental crust (Holliger & Kissling, 1992; Müller, 1977; Musacchio et al., 1998). By using the same rock subdivision as for bulk densities and the same volume proportion between upper, middle and lower crust where the upper part is further divided into unconsolidated sediments, consolidated sediments and crystalline upper crust, (Fig. 14), we obtain average Vp0 of 5.77 km/s (stdev = 0.28) for consolidated sediments of the upper crust, 5.62 kg/s (stdev = 0.28) for crystalline upper crust, 6.12 km/s (stdev = 0.29) and 6.56 km/s (stdev = 0.47) in the upper, middle and lower crust, respectively. While the values for upper and middle crust correspond with values obtained by long-range refraction seismic profiling in the Alpine region (e.g., Waldhauser et al., 1998 and references therein), for the lower part of the crust we must take into account that the mafic and acid components present quite different average velocities (e.g. 6.82 km/s in gabbros, and 5.97 in kinzigites) and an average of the whole lower crust can be strongly affected by the percentages of the mafic vs/acid components. As documented in various refraction seismic models (e.g. Kissling et al., 2006; Ye et al., 1995 and references therein) for the Alpine region and in excellent correspondence with the outcropping lower crust in

the zone Ivrea Verbano (Holliger & Levander, 1994), the continental lower crust is strongly interlayered, with the mafic and ultramafic part accounting for only about half of the volume. Thus the average P wave velocity of lower crust may be estimated as 6.5 to 6.6 km/s and this corresponds very well with the refraction seismic findings.

In Fig. 14 the average velocities for upper middle and lower crust have been corrected for pressure and temperature derivatives considering a geothermal gradient as proposed by Okaya et al. (1996) below the calcareous Alps, and a lithostatic gradient of 16.7 MPa/km for unconsolidated sediments, 21.6 MPa/km for upper and middle crust, 26.5 MPa/km for lower crust and 34 MPa/km for mantle. The derivatives applied for pressure (kms^{-1} MPa^{-1}) and temperature (kms^{-1} $°C^{-1}$) corrections were respectively 0.005 and 0.001 for unconsolidated sediments, 2.12×10^{-4} and 2.00×10^{-4} for consolidated sediments, 8.85×10^{-4} and 2.68×10^{-4} for crystalline upper crust, 5.40×10^{-4} and 4.5×10^{-4} for middle crust and 4.49×10^{-4} and 3.58×10^{-4} for lower crust. It is important to notice that the derivatives for pressure and especially for temperatures are still quite scarce in the database, and the used values are only indicative but might change quite largely once new data will be added to the dbase. Figure 14 clearly shows quite striking similarities between the velocity/depth profile calculated through the averages of bulk density and Vp0 of the dbase and the velocity profile proposed in Müller (1977). It is also noticeable that the contrast of seismic impedances generated at the boundary between i.e. gabbros and stronalites (reflection coefficient R=0.04) or stronalites and kinzigites (R=0.08) or gabbros and kinzigites (R=0.11), here calculated for an average depth of 30 km, correlate very well with the well-known higher reflectivity of the lower continental crust, as, f.e., described by Holliger and Levander (1993) in a conceptual model based on the cross section in the Ivrea Verbano zone.

At present in the dbase only P waves observations are abundant enough to develop statistics and have been used in these calculations.

Regarding the visual representation of the data, we underline that we preferred to plot the intrinsic velocity (V0, see Sect. 3 and Fig. 5) because they are not affected by fractures, they are expression of only the contribution of the solid skeleton of the rock and, therefore, better characterize each rock type. By performing statistics on values collected at room pressure we would document the lithological velocity combined with the maximum effect of porosity and fracturing. Such data does not clearly characterise a rock type because the effect of fractures could have a great impact on these measurements, sometimes larger than the difference between two rock types. Of course, for many applications the void space of the rock, the porosity, is an important property, or it is important to visualize the velocity distribution at shallow depth where porosity is open and plays a particularly important role (e.g., for the in-situ measurements with refraction seismic along the NFP20, see Ansorge & Baumann, 1997). For such case, the dbase offers an abundant collection of measurements at room pressure.

Porosity is also one of the most abundantly collected property (at present the dbase contains 1077 data on absolute porosity). We decided not to plot porosity distribution maps because this property can have quite a large range of values within the same rock type, being more linked to the local depositional history or tectonic environment than to a lithology type. Therefore, data as porosity are collected as point values and a further data treatment should be done to produce porosity maps, in this case not linked to rock types and, therefore, not based on the geotechnical map (Federal Office of Topography, 2006). An example on how porosity variation, both laterally and at depth, can be complex and related to multiple factors is described for example in Aschwanden et al. (2019) for the Muschelkalk, a Middle Triassic formation composed of a dolomitized mudstone, extending below the Swiss Molasse basin at variable depth down to more than 5000 m below the Alpine front. The study underlines how multiple factors such as sedimentary inheritance, diagenesis, various mechanisms of compaction active at different depth, precipitation of minerals from hydrothermal water along faults, contribute to the reduction of porosity with depth. Such complex pictures cannot be captured by statistical analysis over the Muschelkalk formation but deserve more appropriate and focussed studies.

Many other properties in the dbase have been collected only as point data (Fig. 2) and we did not try any statistical treatment, because, as for porosity, there is no direct link to a rock type (e.g. thermal conductivity, which is mainly linked to porosity and fluid content), or because the number of data is at present too low to provide a solid statistic (e.g. magnetic properties; Vs). Examples of graphical presentation of properties for which the number of data allows calculation of statistical distributions are presented in Additional file 1: S5.

6 Conclusions

This project aims to collect, analyse, digitise and reproduce dispersed laboratory data on physical properties of rocks of Switzerland and surrounding regions that carry geological relevance. The final aim is to provide an organized and controlled collection of data, including estimates of uncertainties and links to original data sources, representative of all the main rocks types of a

continental crust. The collection should be able to represent a useful data base for academic studies but also for applicative purposes. It should be open to the wide public and should be able to benefit from input from new data collections.

The SAPHYR dbase centralises, homogenises and sustains otherwise widespread, differentiated and inaccessible laboratory and literature data, and information stored in master theses, and reports issued by Swiss scientific committees, or semi-private data collection. Data are carefully checked for consistency and completeness of information that allows to attribute each data to a geographic location and a specific rock type. The dbase is used to calculate physical properties maps, upon statistical treatment of each data group.

Here we describe as example of presentation of the data, the bulk density and Vp0 maps of Switzerland, as well as the used statistical method to construct these maps from sample data and the methodology behind this approach.

The data collection has been transferred to the Federal Office of Topography swisstopo, with the intent to make the dbase open and accessible online by the swisstopo webpage. In the swisstopo dbase tool there will be physical properties distributions for each lithology group.

The GIS based SAPHYR library should be continuously updated by including new laboratory and literature data and by re-assessing sample characteristics. The more data points included in the database, the more specific lithology groups will form, resulting in an optimised map resolution.

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s00015-021-00389-3.

Additional file 1. Supplementary text and tables to complete the information in the main text and in particular: **S1.** Dbase data literature: list of literature from which physical properties were extracted; **S2.** Lithology list for the SAPHYR lithology groups and corresponding lithology types from the geotechnical map of Switzerland (Swiss Federal Office of Topography swisstopo 2006); **S3.** Anisotropy measurements; **S4.** Dbase of grain density, bulk, density, and Vp0 of the SAPHYR lithology groups; **S5.** Examples of physical properties statistical distribution.

Availability of data and materials
The datasets presented in the current study are available from the corresponding author upon request. The dbase will be in parts available on the portal of the Swiss Federal office of Topography swisstopo.

Declarations

Competing interests
The authors declare that they have no competing interests.

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