

## Geochemical database of Japanese islands for data-driven science: problem and solution of published domestic data

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Geochemical database of Japanese islands for data-driven science: problem and solution of published domestic data

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Recent progresses in the earth science have introjected a data-driven approach, which deals with a huge amount of high-dimensional data. Gathering several kinds of data, e.g. major element composition, trace element composition and isotopic ratio, with GPS-position data can provide a better understanding of the geological phenomena. For such kind of big data science, several databases covering geochemical, geochronological, and petrological data are constructed and available on the internet, such as PetDB, SedDB and GeoRoc. These databases are constructed by collecting a number of published data. However, the existing international databases are based on the collection of studies in the international publication of societies and projects. The data in the publication of non-international journals and domestic institutes are rare in the international datasets. As a result, compositional data of rocks from Japan arc are not fully covered by these databases. Therefore, we construct a geochemical database for those published in the Japanese language and provided in domestic journals.

We collected literature including geochemical data of Japanese islands published from 1980's to present. During the data compilation, we took special care of position data. Position data are crucial for understanding geographical distribution of geochemical components, and also important to estimate geo-neutrino flux from the crust. Increasing availability of handy GPS logger provides easy access to the standardized position data. However, many of the published geochemical data still lack GPS-position data, and of course, old publications provided position information only by map images. We use Google Earth for reading position data from map images. The geological map of papers including sampling points is projected on Google Earth. Latitude, longitude and altitude of the sampling points on the map are obtained based on the coordinate system on the Google Earth.

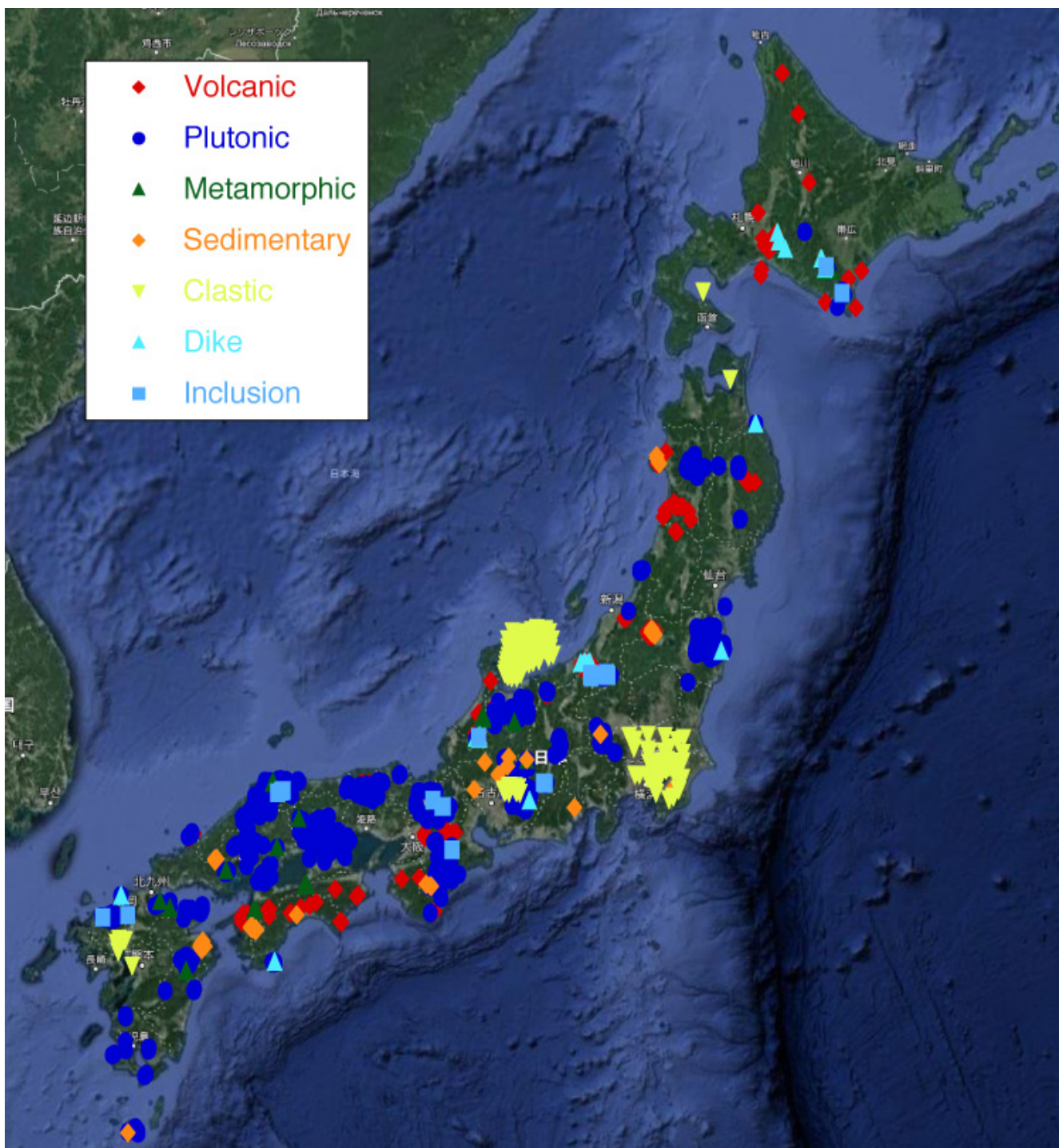
The articles published in 1980's and 1990's are usually provided as scanned PDF of a printed paper, and thus, tables are provided as images. Furthermore, some journals still provide tables as images. Despite the developed OCR (optical character recognition) technique, the transformation of image tables to numerical data requires checking by eyes of a human. In addition, pdf files provided by some publishers (e.g. J-stage) are protected and data in the file are not directly available for computer-based treatments. To overcome these problems, we have edited this new geochemical database.

Our database covers several rock types including volcanic rocks, plutonic rocks, sedimentary rocks, metamorphic rocks, and so on, and from Hokkaido to Kyushu Island (Figure 1). The main purpose of our database is “basement characteristics” of the Japanese islands: therefore, we pay great attention to collecting data mainly plutonic, metamorphic and sedimentary rocks. One of the important points of our database is covering rock types other than the volcanic rocks, because many parts of the existing geochemical database is focused on volcanic rocks, and metamorphic and sedimentary rock data are rare.

The compiled database is going to be published under the appropriate science commons license, although the idea of *science commons* has not been widely accepted among the geoscientists (Watanabe & Noguchi, 2010). We will provide information about our database on the website (<http://dsap.jamstec.go.jp>).

This database will be used to multiple purposes, such as multivariable statistical analyses (Iwamori et al., 2017), estimateon of the average crustal compositeon (e.g. Togashi et al., 2000), geographyc statistical analyses and the estimateon of the crustal geo-neutrino flux (Enomoto et al., 2007).

Keywords: position data, published geochemical data, Basement of Japanese islands, geochemical database



# Geochemical characteristics of paleo-tsunami deposits using multiple classification analysis

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Cataloguing and assessing tsunami records are important for long-term tsunami prediction and for tsunami-hazard mapping. However, like on a number of other tsunami-susceptible coastlines, historical records of tsunamis are too short to develop a predictive chronology of events. Understanding the geochemical characteristics of tsunami sediments is significant for revealing the mechanisms of tsunami inundation. Principal component analysis (PCA) can be used to extract geochemical features of tsunami sediments. It is one of the most pervasive multivariate analysis techniques which can be used for extracting the hidden structure and pattern from high-dimensional data in various fields of natural and social sciences. We conducted field surveys in February and March 2016 in Wakabayashi, Sendai City. The sedimentary sequence contained a disturbed sandy soil at the top, overlying a mixed layer with the To-a and Jogan tsunami deposit, as well as characteristic sand layers at about 50 cm, 103-113 cm and about 140 cm depth. The core was analyzed using an ITRAX X-ray fluorescence core scanner, which provides high resolution semi-quantitative elemental data, as well as photographic and radiographic images. Major elements (Si, K and Ca etc) showed high counts at 100~110 cm depth, while the distribution of minor and trace elements (Zn, Cr and Zr etc) was more variable. The Mo ratio (Mo<sub>coh</sub>/Mo<sub>inc</sub>) which is an indicator of organic content was, as expected, lower in sandy layers than in the peat. The PCA was performed using normalized counts of 17 major elements and minor/trace elements. The PAC was showed geochemical characteristics of tsunami deposits in a comprehensive fashion. The above 3 factors, such as PC1, PC2 and PC3 can explain the processes that contribute to the chemical variations. These results and the other geological evidences can be useful for understanding the mechanism of the tsunami indentation.

Keywords: tsunami deposits, multiple classification analysis, geochemical characteristics

# Sparse feature selection for clustering and sample-wise distance, with application to geochemical data

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Many geochemical data, such as multiple samples from the single volcano or rock suite, and the multipoint-local analysis in one sample, are the assemblage of many samples each of which has high dimensional composition data. In order to extract geochemical process hidden in the rock samples, it is necessary to conduct a data-driven multivariate analysis of high dimensional data consisting of multivariate-multi samples. However, most previous geochemical studies have been carried out at low dimensions, such as only the relationship between several elements, or focusing on only a few specific samples. Furthermore, data analyses were carried out with giving some specific assumptions such as chemical compositions of some end-member components. Furthermore, data distributions and its shape are not fully utilized in previous studies, although the rock formation process should be reflected in the shape of the data distribution made by many samples. It is expected that more geochemical information can be extracted from the geochemical data by analyzing the distribution of data in multidimensional space quantitatively.

In order to analyze such kind of data, we considered the "distribution" defined by the observation values of the series of samples or multiple analyses. We measured the distance between the distributions. The distance between distributions is derived by a nonparametric method which does not assume any specific probability distribution. The distance corresponding to each feature quantity is defined. The total distance is defined by the weighted sum of "element distances". By using clustering with this weight and further selecting features by imposing sparse constraints on the weights, we can calculate the distances between sets and the quantities characterizing distances (in the case of this study, the elemental species and the specific isotopic ratios).

The advantages of this method are,

1. It enables us to determine variables characterizing the distance,  
and

2. It is unnecessary for all samples to have analytical values of all elements with this method.

Using rock chemical composition database "petdb" (<http://www.petdb.org>), compositional data of 3988 MORB samples, up to 49 elements (including 5 isotopes and 10 major elements) was compiled and used for analysis. Based on its spatial distribution, MORB was grouped into several clusters and chemical compositions and distances between the clusters are compared. Elements or isotope ratios that characterize the spatial variation and the distances between the clusters were obtained using this method. As a result, MORB is clustered into the east-west hemisphere. Sr isotope ratio was found to be most important as an amount characterizing the spatial variation of MORB. Clustering of this east-west hemisphere is consistent with the structure shown by Iwamori and Nakamura (2015). Since the Sr isotopic ratio is sensitive to the amount of recycled material in the source mantle (e.g., Hoffman, 1997; Albarede, 2009), it is suggested that the distribution of recycled material of the subducted slab is systematically different between the east and western hemispheres.

Keywords: MORB, Machine learning, Geochemical data

## Cluster analyses for volcanic pyroclasts using grain shapes

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Our motivations for this study are: 1) classify volcanic ash using statistical techniques, and 2) identify eruption styles from parameterized grain shape of pyroclasts. One of the extractable factors which we can infer eruption styles and mechanisms is grain morphology of ejected pyroclasts. They would tell us characteristics of magma vaporization and fragmentation (e.g., Heiken and Wohletz, 1985). Numbers of researchers have been tried to parameterize grain shapes and discussed its formation and fragmentation story. Thanks to the development of grain analyze instruments and techniques, we can parameterize visuals (shape and intensity) for thousands of grains easily in short time. Previous studies have applied an automated particle analyzer (APA) for grain shape of volcanic ash. Leibrandt and Le Pennec, 2015 tested several measurement conditions, then presented an efficient protocol. Using this protocol, Liu et al., 2015 compared the characteristics of grain shape parameters among components (dense, vesicular, and shards) and eruption styles. Thus, we are closing to know eruption style and characteristics by grain shape analysis using the APA. To simplify this system, first we should test this method in simpler cases, i.e., monogenetic volcanoes.

This study verified several patterns of clustering for volcanic pyroclasts. We used 47 samples which were collected in several places of Japan and Iceland. These pyroclasts were formed in three types of monogenetic eruptions; magmatic, phreatomagmatic, and rootless. Each sample consist of more than 100 grains. We measured grain shapes and intensities using an APA: Morphologi G3STM (Malvern InstrumentTM) in AIST. Using parameterized grain data, we performed cluster analyses on R software (R Core Team, 2016) with the hierarchical procedure (Ward's method) and Euclidean distance. In test analysis using analog grains, it is found that scaling of each parameters before clustering are unnecessary. We performed clustering in 2 steps; make grain types and clustering among samples using percentages of each grain type. In this presentation, we will show processes and results of our clustering, and consider better way to apply the cluster analysis to natural volcanic products.

Keywords: cluster analysis, pyroclast, grain shape

## Fast and precise quantitative compositional mapping and its application to the Nové Dvory ultra-high pressure eclogite.

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Rocks often show chemical inhomogeneity in various scales owing to layers, veins, and so on. To evaluate such inhomogeneity, quantitative compositional mapping would be a powerful tool, since ordinary EPMA quantitative analysis takes large time (> 1 min/spot). Lanari et al. (2014) established a fast analytical technique by combining qualitative mapping (> 100 msec/px) and quantitative analyses (ca. 20 spots/phase). To make quantitative map data, they performed mode analysis for the map data by k-means cluster analysis, calibrated the relationship between map intensity and real concentration for each element of each phase, and applied the calibration to the modal composition. Their technique saves great time, but the analysis still takes long time for the large samples due to recommended analytical conditions of spatial resolution (< 10  $\mu$ m pixel size) and dwell time (> 100 msec/px) for the mapping, e.g. 55 hours for the area of 100mm<sup>2</sup>. This study aims to shrink analysis time further.

The mapping time is proportional to the spatial resolution in  $O(N^2)$  and the dwell time in  $O(N)$ . Thus, decreasing the spatial resolutions saves more time than decreasing the dwell time. Yet, it increases the amount of pixels containing multi-phases, especially when a mapping area contains fine-grained minerals. This problem can be solved by modifying methods of (a) clustering, (b) estimating calibration curves, and (c) applying calibration curves after Lanari et al. (2014).

(a) The soft-clustering is preferred to the hard-clustering (k-means) because it explains proportion of phases in pixels. Since compositional distribution of the map data can be approximated by mixtures of Poisson distributions, this study employed the mixture-Poisson-distribution-model clustering.

(b) Calibration curves for trace components of phases, i.e. elements not included in the stoichiometry, tend to contain large errors. For such components, calibration curves are determined by using all phases.

(c) Composition of a pixel containing various phases is obtained from a weighted mean of concentrations estimated by the calibration curves of each phase, which is weighted by the modal composition of the pixel.

The newly developed technique is applied to the Nové Dvory eclogite, containing pyroxene-rich layer (Layer-P) and garnet-rich layer (Layer-G) in mm-scales. Garnet (Grt) between these layers has Mg-richer core (ca. Fe<sub>23</sub>Mg<sub>56</sub>Ca<sub>21</sub>) than Grt in Layer-G (c.a. Fe<sub>30</sub>Mg<sub>32</sub>Ca<sub>38</sub>), and both Grt show similar rim compositions (ca. Fe<sub>28</sub>Mg<sub>44</sub>Ca<sub>28</sub>). The core compositions probably reflect the inhomogeneity of the protolith (Yasumoto & Hirajima, 2015), though the cause of the inhomogeneity is unclear. Compositions of these layers are estimated by our technique. Qualitative mapping is done in the area of 10 mm \* 33 mm with 20  $\mu$ m pixel size and 120 msec dwell time, taking ca. 55 hours. Total wt% of Layer-P is improved by the technique of ours (97 wt%) than Lanari et al. (2014) (91 wt%), while that of Layer-G are comparable (97 wt% and 98 wt%, respectively), probably because fine-grained texture of Layer-P compared to Layer-G.

The estimated compositions show Mg-Cr-rich ( $XMg = Mg/(Mg+Fe) = 0.79$ ; Cr<sub>2</sub>O<sub>3</sub> = 0.14 wt%) for Layer-P and vice versa for Layer-G ( $XMg = 0.64$ ; Cr<sub>2</sub>O<sub>3</sub> = 0.07 wt%). One possible explanation is that Layer-P and G are metamorphosed from pyroxene-rich and plagioclase-rich layers of gabbro, respectively. However, a large difference in XMg of Layer-P and G is unlikely for the gabbro-origin. Cr content of both layer and Mg/Fe ratio of Layer-P are also unlikely high (e.g. general gabbro: Cr<sub>2</sub>O<sub>3</sub> < 0.01 wt%; XMg  $\approx$  0.65). Field occurrence shows dominance of Layer-G with minor Layer-P, indicating that Layer-P was crystallized from pyroxenite melt intruded to gabbroic host (Layer-G), and Layer-G partially reacted with the melt. This idea

is supported by presence of pyroxenite melt intrusions ( $X_{Mg} = 0.80-0.91$ ;  $Cr_2O_3 = 0.2-1.7$  wt%) in peridotite which hosts the study eclogite (Svojtka et al., 2016).

Keywords: Quantitative Compositional Mapping, Rock-Melt Reaction Textures, UHP, Eclogite

# AN EVALUATION OF THE APPLICATION OF X-RAY MICROSCOPY IN UNDERSTANDING GOLD LOSSES IN TAILINGS

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The extractive metallurgy of gold is largely controlled by mineralogical factors such as the presence of refractory gold, particle size, gangue mineral associations, presence of preg-robbbers, oxygen and cyanide consumers, and locking characteristics in base metal sulphides.

Light microscopy and automated mineralogy techniques are regularly used to characterise the effect of these variables on gold recovery. However, despite their widespread application there are a range of limitations when grades are low. Typically, the analysis of low-grade samples requires the preparation and analysis of numerous polished blocks. This is often costly and time consuming, with complexities regarding analysing statistically representative particle quantities and problems overcoming stereological bias. This is compounded by the “nugget” effect and high tenor nature of gold mineralisation.

X-ray Microscopy techniques have the potential to overcome many of these problems, in particular the statistical representivity of analysis, removing stereological bias and effectively locating phases that are present in ultra-trace proportions. In this paper we outline the potential benefits of employing X-ray Microscopy (XRM) in characterising gold losses from a typical Cu-Au porphyry project, which were illusive in 2D based analysis. The talk will also outline additional application areas of XRM within the extractive value chain.



## Progressive evolution of the whole rock composition during metamorphism revealed by machine learning technique

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Geochemical evolutions with respect to the major components of the metamorphic rocks during the subduction-related metamorphism are documented on the basis of multivariate statistical analyses applied for mapped metamorphic rocks collected from the Sanbagawa metamorphic belt in central Shikoku, whose metamorphic conditions range from the pumpellyite-actinolite to epidote-amphibolite facies. Recent progress of computational and information science provides a number of algorithms revealing a hidden structure of large datasets. This contribution applied *k*-means cluster analysis (KCA) and non-negative matrix factorization (NMF) to a series of metapelites, which is the main lithotype of the Sanbagawa metamorphic belt. The analyzed dataset contains 235 sample with 14 elements accumulated from the literature. As a result, we obtain five clusters in KCA and four endmembers for NMF which successfully explains compositional variations of the studied dataset.

The result of KCA clearly shows that the chemical compositions of the metapelites are different between the western part (Besshi area) and eastern part (Asemigawa area) of the studied dataset. In the western part of the studied dataset, clusters show a good correspondence with the metamorphic grade. In the higher metamorphic grade part, a monotonous decrease in SiO<sub>2</sub> and Na<sub>2</sub>O and an increase in other components are detected. On the other hand, the compositional change with the metamorphic degree is less obvious in the eastern part. Endmember decomposition using NMF revealed that the evolutionary change of the whole rock composition correlated with the metamorphic grade is approximated to a stoichiometric increase of garnet-like component in the whole rock composition. This phenomenon could be related to the precipitation of garnet and effusion of other components during progressive dehydration. Thermodynamic modeling considering the evolutionary change of the whole rock composition predicted followings: (1) the lower-grade whole rock composition prefers the crystallization of garnet at the conditions of the garnet zone while biotite becomes stable together with garnet in higher-grade whole rock compositions at the same PT conditions, (2) the higher-grade whole rock composition can retain more H<sub>2</sub>O than the lower-grade one. These results indicated the mechanism suppressing the dehydration at the high-pressure metamorphic conditions. Perhaps such kind of mechanism should be considered in the forward modelling in treating the fluid cycle in subduction zones, though quantitative model has not been established yet.

Keywords: machine learning technique, Sanbagawa metamorphic belt, subduction zone, pseudosection analysis, material cycle

## Automatic detection of Martian dust storm's area using basis images extracted by Independent Components Analysis

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This study was performed for automatic detection of Martian dust storm's area from satellite images of Mars, using basis images extracted by Independent Components Analysis (ICA). Normalized images are divided into several patch images with the predetermined size. A classifier is trained by coefficients which are multiplied by the basis to reconstruct the patch images based on the basis images. When we detect dust storm's areas from test images, we evaluate whether a target patch is included in a dust storm or not, shifting the target patch horizontally and vertically by one pixel. Then, a pixel may be included in many patch images. The pixel is regarded as included in a dust storm if more than half of patches including the pixel are recognized as the dust storm by the classifier. Precision, recall and F-score are used for evaluation of the method, and F-score is 0.87. The method developed in this study can accurately detect dust storm regions from Mars images.

Keywords: Mars, dust storm, Independent Components Analysis

# High precision hydrothermal plume survey based on multi-sensor data processing

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To date, multi-beam echo sounder (MBES) equipped on Research vessels and AUVs has been widely accepted as a powerful tool for detecting interception of any rising, buoyant hydrothermal plumes, without water sampling (Nakamura et al., 2015). Although utilization of water column sonar data enabled us to achieve certain results, to find new vents, this approach is not sufficient to distinguish gas seeps and hydrothermal vents, and moreover, it is inadequate to determine hydrothermal plumes with a low gas content. To improve efficiency and accuracy of exploring hydrothermal plumes and to understand their properties, we use multi-sensor data such as temperature, turbidity, redox potential, and methane concentration. These sensors were equipped on AUV Urashima, which was programmed to fly at an altitude of ~200 m above the seabed, at an average speed across the seafloor of ~1.3 m/s. An area of 2000 m x 5000 m on the seafloor can routinely be surveyed, at 400 m line spacing, during a single AUV Urashima dive. In this presentation, we will overview oceanographic, chemical and acoustic sonar data obtained during AUV Urashima Dives 217, 250, 251, and 252 in the Okinawa Trough, and will introduce data-driven analytical techniques to determine chemical properties of the water masses, and make a comparative review of 3 discrete hydrothermal fields. Each hydrothermal field has different features: i) Yokosuka Field, the highest temperature vent-site on record in the Okinawa Trough (364.1°C at 2183 m depth), shows strong water column acoustic reflections and consistently detectable sharp peaks in turbidity, redox potential, and methane concentration. ii) Futagoyama Field is characterized by its gas seeps, strong water column acoustic reflections, and little change in turbidity and redox potential. iii) hydrothermal field off-Kume Island, which includes at least 9 active hydrothermal vents, is characterized by its acoustically invisible plumes, low H<sub>2</sub>S content, as well as sharp peaks in turbidity, redox potential, and methane concentration. These case studies will provide an insight into the feature of each hydrothermal activity, and ensure much more efficient use of deep-submergence assets such as human occupied vehicles and remotely operated vehicles during follow-on studies.

Keywords: hydrothermal, AUV, Okinawa Trough, machine learning

# Chemostratigraphic analysis on the Middle Triassic (Anisian) Oceanic Anoxic Events

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Superanoxia across the Permian Triassic boundary, which has a long duration from the late Middle Permian to the early Middle Triassic (about 20 million years), is globally recognized and debated well in the context of the end Permian mass extinction. However, few studies focus on the integrated decoding of the recovery processes in the Anisian from Superanoxia because of limited application of geochemical proxies. To reconstruct the interactions between the environmental factors from multi elemental data, principal component (PC) analysis was performed on the Middle Triassic chemostratigraphy of the pelagic deep sea sequence in the Mino belt, central Japan. Major and trace element concentrations in the samples were determined by X-ray fluorescence spectrometry (XRF). Before PC analysis, the data matrix (438 samples and 20 elements) was normalized for constant sum. As a result, six PCs were statistically accepted and capture 77% of the total variability. The sedimentological interpretations for the components were as follows. PC1 represents the chemical weathering intensity of terrigenous materials. From the time series data of the PC1 scores, a frequency analysis detects dominant sedimentary cycles similar to the Milankovitch cycles. PC2 is the direction along the enrichment of redox sensitive elements. These records indicate astronomical driving force behind the oceanic redox evolution during the Middle Triassic. PC3 might be related to the deposition of the siliceous claystones called the Toishi type lithofacies. PC4 explains the depletion and accumulation of ferromanganese oxides precipitated from seawater across the anoxic event intervals. PC5 might be interpreted as mixing with heterogeneous materials because the scores shows no systematic variations with the lithostratigraphy and a sample with an anomalously high score has a remarkable chemical composition. PC6 might reveal the abundance of biogenic materials. Further non parametric approaches and conodont biostratigraphic correlations would lead to superior paleoenvironmental reconstruction by predicting more precise sedimentological components.

## Change point in log-periodic power law time series of atmospheric radon concentration

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Radon is a radioactive element which belongs to uranium series with a half-life of about 3.8 days. Radon ( $^{222}\text{Rn}$ ) is produced by alpha decay of radium ( $^{226}\text{Ra}$ ). Anomalies in atmospheric radon concentration related to earthquake occurrence have been reported. For example, it has been reported that anomalous increase in atmospheric radon concentration observed in Kobe Pharmaceutical University before 1995 Kobe earthquake (Yasuoka and Shinogi, 1997). It is considered that stress change in the crust causes exhalation of radon from the ground surface resulting in anomalous atmospheric radon concentration (Yasuoka et al., 2009). Moreover the increase before the earthquake according to the log-periodic power law has also been reported (Yasuoka et al., 2006). The log-periodic power law is one of the critical phenomena models, and it is characterized by the fluctuation (logarithmic periodic oscillation) toward the critical point. In addition to the case of atmospheric radon concentration, the power law is also reported in cumulative benioff strain (Newman et al., 1995), chloride ion concentration in ground water (Johansen et al., 1996) and relative ground level (Igarashi, 2000). For fitting the power law model to observed data, it is necessary to analyze by nonlinear least squares method and to define a period for estimating parameters of the model. In previous studies, the periods were selected arbitrarily (e.g., Igarashi, 2000). In this research, we apply a recurrence plot to evaluate nonstationarity of the data to define the fitting period as a non-change of data structure.

We used atmospheric radon data observed at Fukushima Medical University (FMU) from January 2003 to February 2011. As a result, structural change in data of cumulative atmospheric radon concentration after the 2008 Ibaraki-ken Oki earthquake ( $M_w$  6.8) was revealed. The power law observed in the cumulative atmospheric radon concentration diverges towards the 2011 Tohoku Oki earthquake. Regarding the 2011 Tohoku Oki earthquake, an increase in the power law has also been reported in cumulative benioff strain (Xue et al., 2012). Cumulative atmospheric radon concentration observed at FMU and benioff strain (Xue et al., 2012) with log-periodic power law seem to indicate critical phenomena of the 2011 Tohoku-Oki earthquake. Beside, application of the recurrence plot to Earth science data has a benefit to know the structural change-point in nonstationarity data.

Keywords: atmospheric radon concentration, earthquake precursor events, log-periodic power law, recurrence plot

# Modelling nitrous oxide emissions in a wheat-maize system of North China Plain

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Concentrations of atmospheric nitrous oxide (N<sub>2</sub>O), a potent greenhouse gas, has been continuously increasing and cropland soils are one of the largest sources of N<sub>2</sub>O. Variations in environmental and anthropogenic alterations have great impacts on both the frequency and magnitude of N<sub>2</sub>O emissions. Based on the measurements from a wheat-maize system of North China Plain, we parameterized the APSIM model which was initially developed in Australia, for simulating nitrous oxide emissions under different agricultural management practices. After calibrating one of the key parameters, i.e., fraction of N<sub>2</sub>O lost in nitrification ( $k_2$ ), the results showed that the model can well capture the daily nitrous oxide fluxes under different nitrogen fertilization treatments, but underestimated some large peak fluxes. By pooling all data together, the calibrated APSIM model also showed a good performance in representing the cumulative N<sub>2</sub>O emissions with various treatments at both annual and finer (monthly and daily) time scales.

# Seismic wavefield imaging in the Tokyo metropolitan area, Japan, based on the replica exchange Monte Carlo method

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Earthquakes sometimes cause serious disasters not only directly by ground motion itself but also secondarily by infrastructure damage, particularly in densely populated urban areas. To reduce these secondary disasters, it is important to rapidly evaluate seismic hazards by analyzing the seismic responses of individual structures due to the input ground motions. Such input motions are estimated utilizing an array of seismometers that are distributed more sparsely than the structures.

We propose a methodology that integrates physics-based and data-driven approaches in order to obtain the seismic wavefield to be input into seismic response analysis. This study adopts the replica exchange Monte Carlo (REMC) method, which is one of the Markov chain Monte Carlo (MCMC) methods, for the estimation of the seismic wavefield together with one-dimensional local subsurface structure and source information. Kano et al. (2017) conducted numerical tests, showing that the REMC method was able to search the parameters related to the source and the local subsurface structure in broader parameter space than the Metropolis method, which is an ordinary MCMC method. The REMC method well reproduced the seismic wavefield consistent with the true one. In contrast, the ordinary kriging, which is a classical data-driven interpolation method for spatial data, was hardly able to reproduce the true wavefield even at low frequencies. This indicates that it is essential to take both physics-based and data-driven approaches into consideration for seismic wavefield imaging.

Then the REMC method is applied to the actual waveforms observed by a dense seismic array MeSO-net (Metropolitan Seismic Observation network), in which 296 accelerometers are continuously in operation with several kilometer intervals in the Tokyo metropolitan area, Japan. The estimated wavefield within a frequency band of 0.10–0.20 Hz is absolutely consistent with the observed waveforms. Further investigation suggests that the seismic wavefield is successfully reconstructed at frequencies up to 0.30 Hz in terms of the variance reduction (VR), but the VR gets rapidly worse in higher frequencies. On the other hand, the velocity response spectra of the reconstructed wavefield show good agreement with the observations even in higher frequencies up to 1.0 Hz in terms of the combined goodness-of-fit (CGOF), which measures the misfit in the velocity response spectra. In summary, the proposed seismic wavefield imaging based on the REMC method is effective < 1.0Hz, which is enough to evaluate large-scale seismic hazards in almost all infrastructures.

Keywords: MeSO-net, Seismic Wavefield Imaging, MCMC

# Stochastic modeling of temperature extremes over continental US and Canada

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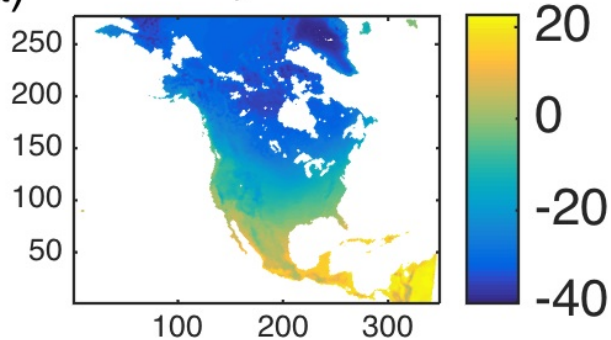
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An extremely statistically accurate, essentially bias-free empirical emulator of atmospheric surface temperature is applied for meteorological risk assessment over the domain of continental US and Canada. The resulting prediction scheme achieves an order-of-magnitude or larger gain of numerical efficiency compared with the schemes based on high-resolution dynamical atmospheric models, leading to unprecedented accuracy of the estimated risk distributions. The empirical model construction methodology is based on our earlier work, but is further modified to account for the influence of large-scale, global climate change on regional US weather and climate. The resulting estimates of the time-dependent, spatially extended probability of temperature extremes over the simulation period can be used as a risk management tool by insurance companies and regulatory governmental agencies.

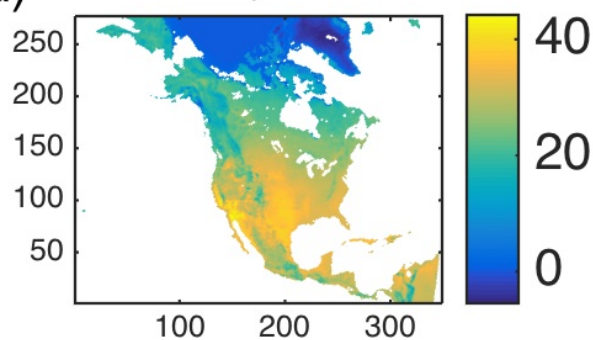
Keywords: Stochastic modeling, Temperature extremes, Risk assessment



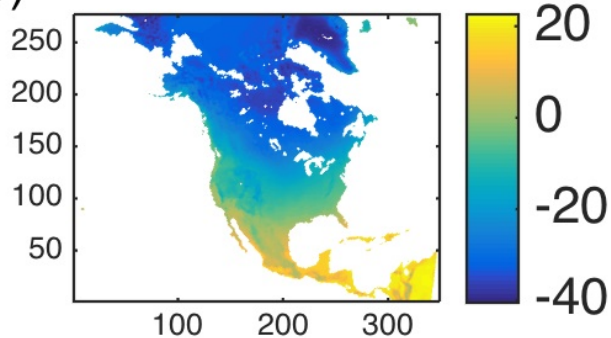
(a) T2 2.5%, DJF Obs



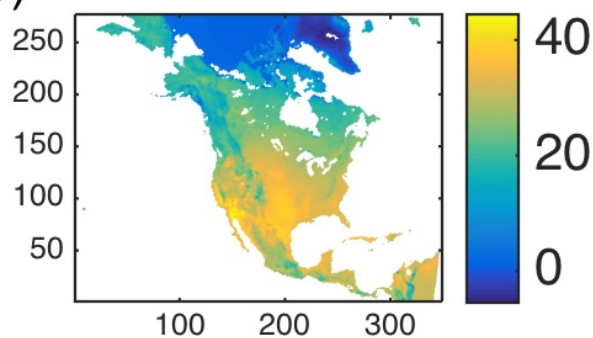
(d) T2 97.5%, JJA Obs



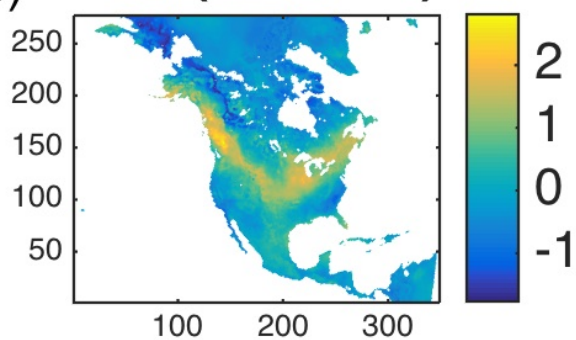
(b) T2 2.5%, DJF Sim



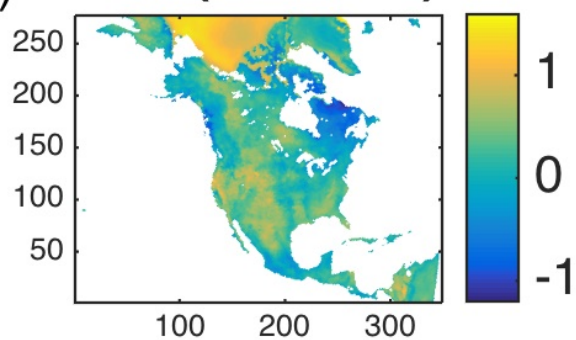
(e) T2 97.5%, JJA Sim



(c) Diff. (Sim-Obs)



(f) Diff. (Sim-Obs)



# Data driven analysis for a prediction method of arsenic adsorption to soils

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Arsenic is a trace element that is toxic to plants, animals and humans. Arsenic moved to the surface of the earth via ground water can cause skin diseases. Thus it is important to predict the amount of arsenic in soil. However, it is too difficult to describe the absorbed amount of arsenic in soils because in the surface in soil it occurs as and that forms two types of complexes (inner-sphere complex and outer sphere complex), which we can't distinguish. We used regression analysis as a new predictive method for arsenic adsorption. Arsenic adsorption tests were conducted using nine type soils and applying Freundlich isotherm. At the same time, we measured the 13 characteristic values of soils (pH, EC and the content of Na, Mg, Al, Si, P, S, K, Ca, Ti, Mn and Fe). Finally, simple and multiple regression analysis were used as a method of data driven analysis. The simple regression was applied to relate all parameters to Freundlich constant and exponent. In multiple regression, we calculated all combination from measured 13 parameters. They were also applied to relate Freundlich constant and exponent are associated. The best model expression was selected from calculated 91 formulas by using the coefficient of determination and Student's t-test., which proves the effectiveness of regression coefficients. The best model formula, which showed 95% reproducibility, consisted of the EC value, and Ti and Al content. This indicates that arsenic adsorption by soils is mainly arsenic competing with salts, and the occurrence of titanium iron and an Al-bearing mineral. We showed the availability of data driven analysis for predicting arsenic adsorption.

Keywords: soils, adsorption, multiple regression analysis, arsenic

# Multivariate analysis on major element compositions of Apollo 16 impact melt

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Impact melt rocks and clasts from Apollo 16 landing site record heavy bombardment history called the Late Stage Heavy Bombardment (LHB) supported by impact reset ages of the impact melt rocks clustering around 4.1–3.8 Ga [e.g. 1-3]. However, the age clustering might include a sampling bias; for example, some rocks could record the same impact event. Therefore, attempting to identify and characterize individual impact events is important to understand LHB. Bulk composition is one of the important factors to identify the impact event. Bulk chemical composition of impact melt thought to maintain almost average composition of pre-impact target material. Classification of Apollo 16 impact melt has been established using trace element compositions using Sc and Sm [4]. Based on the method, impact melts are classified into major 4 groups, Group 1 to 4. However, most of the impact melt especially small mass samples does not have such information. Therefore, we are developing a new classification scheme using only major element compositions.

We have compiled 330 published data of major, minor, and trace element compositions of Apollo 16 impact melt rocks and clasts [e.g. 4-9]. We selected samples which have 9 major and minor element data (Si, Ti, Al, Fe, Mg, Ca, Na, K, and Cr) and have been already classified by conventional method using trace element information (95 total data). We conducted principal component analysis (PCA).

Our PCA results indicate a difference between mafic and felsic impact melt rocks, although sub-types of Group 2 melt are widely distributed. PC1 distinguishes between mafic and felsic impact melt; more specifically, felsic melt is distinct from mafic melt relatively rich in Fe and/or Mg and poor in Al, Na, and K (wt.%). These elemental compositions have good correlation with PC1 (correlation coefficients are -0.98 and 0.99 respectively for Fe+Mg and Al+Na+K). In addition, our work shows PC2 results correlating with the Mg/Fe weight ratio (correlation coefficient is -0.81; Fig. 2). When we plotted Al+Na+K (wt. %) and Fe/Mg (weight ratio) of Apollo 16 impact melt rocks, the plot has similar trends when compared to the PCA-based trends, although the y axis (PC2 and Fe/Mg) is slightly different. Hence, this plot is also useful in the identification of impact melt types using only 5 major elements (Al, Na, K, Fe, and Mg).

Our PCA results indicate that Apollo 16 impact melt rocks can be statistically classified by using only 9 major elements, as well as trace element abundances. Moreover, our results indicate that impact melts can also be classified by using 5 elements by plotting Al+Na+K and Mg/Fe.

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Keywords: Bulk composition, Lunar samples, Impact melt

## Trans-dimensional imaging of random velocity inhomogeneity at southern Ryukyu arc

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Precise imaging of randomly inhomogeneous structure is essential to describe wave scattering processes of high frequency seismic waves. Recent studies have constructed a fundamental basis of 2D or 3D imaging of power spectral density of random velocity inhomogeneity (e.g., Takahashi et al. 2013). Yet, it is difficult to know how small-scale spatial variations of random inhomogeneities can be extracted from observed seismic wave data. Here we used the reversible Jump Markov chain Monte Carlo (rjMCMC) (Green 1995) to achieve an adequate spatial-resolution imaging of random inhomogeneity. The rjMCMC is a framework of trans-dimensional parameter-sampling under a target distribution. Under the Bayesian framework, we can use this method to solve inverse problems of which number of unknown parameters is variable. In this study, a study area is partitioned into discrete Voronoi cells. A parameter sampling under a posterior probability is conducted with changing number and spatial layout of Voronoi cells, and unknown parameters in cells. Ensemble average of MCMC samples around the maximal posterior would be an optimal result with an adequate spatial resolution. Regularization term for this inversion is defined as a difference between the maximal and minimal values of power spectral density at a large wavenumber. This regularization is a relatively weak constraint, but gives stable reconstructions of original structures in synthetic tests.

We applied this method for S-waves data (4-8Hz, 8-16Hz and 16-32Hz) recorded at southern Ryukyu arc, Japan. Seismic stations consist of 30 ocean bottom seismographs and 6 onshore stations that were temporary deployed for 3 months. Inversion result shows two significant anomalies. One is a strong inhomogeneity in the mantle wedge beneath islands at 30-40km depth. This anomaly, however, shows no clear correlation with other geophysical observations. Another one is imaged beneath a submarine volcano off the southern Ryukyu arc. This inhomogeneity has a gentle spectral gradient at large wavenumber. Similar inhomogeneity was commonly observed in other volcanic rock areas, and then this anomaly may be related magma inclusions. Stable extraction of these anomalies is mainly because of the rjMCMC and weak regularization term. We may say that the rjMCMC is an important basis for precise imaging of underground structures.

# Si-metasomatism during sea floor serpentinization and estimation of its kinetic parameters

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Water-rock interaction is dominant process at the Earth surface and its kinetics is important for understanding geological, climatic, and biological process of the planet. Kinetic parameters of chemical reaction were usually determined by laboratory experiments; however, due to its sparseness and noise, estimating exact parameter is often difficult. To estimate the parameters exactly, machine-learning algorithm were proposed (Omori et al., 2016): however, such machine-learning algorithm for water-rock interaction has not been tested with real experimental data.

In this study, we applied machine-learning algorithm to extract the kinetic parameter of water-rock interaction. Serpentinization is representative hydration process at slow-spreading ridge and play crucial roles on rheological, magnetic, seismic and thermal properties of sea floor. Hydrothermal experiments (230-degree C, 2.80MPa) were carried out in olivine (Ol)-quartz (Qtz)-H<sub>2</sub>O system, as analogues of crust-mantle boundary. By using unique tube-in-tube type hydrothermal experiments vessel, spatial and temporal data were obtained.

After the experiments, the mineralogy of the reaction products in the Ol-hosted region changed with increasing distance from the Ol-Qtz boundary, from talc to serpentine + magnetite. On the other hand, in Qtz-hosted region, talc was also formed. Talc zone was formed 1.0 mm from the boundary in Ol-hosted region, whereas it also formed 0.5 mm from the boundary in Qtz-hosted region.

The observed mineral distribution was modeled by reaction-diffusion equation. To model our experiments, we set eight reaction rate constants; diffusion constant for SiO<sub>2(aq)</sub> and rate constants for olivine→talc, olivine→serpentine, olivine→brucite, serpentine→talc, talc→serpentine, serpentine→brucite, and brucite→serpentine. Firstly, Markov Chain Monte Carlo (MCMC) method were used to calculate the rate constants. This method was tested with artificial data and estimates the true value of kinetic constants with <0.5 % error. However, application of MCMC method to experimental data failed in estimating kinetic parameters, probably because the system studied here is expected to have several local minima. Here, to overcome this problems, we use an optimization algorithm of the exchange Monte Carlo method (Hukushima and Nemoto, 1996) and rate law during serpentinization will be discussed.

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Keywords: Serpentinization, optimization, reaction-diffusion system, Serpentine

## Impact of COSMIC GPSRO assimilation on Indian summer monsoon simulation using variable resolution LMDZ5-DART data assimilation system

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Impact of assimilation of COSMIC GPS radio occultation (RO) data in simulating mean monsoon circulation and rainfall of Indian summer monsoon (ISM) 2015 will be examined in this study using the newly developed LMDZ5-DART ensemble based data assimilation system. The LMDZ5 model is an atmospheric component of the IPSL global model, which has the capability to generate denser grids over an area of interest using coordinate stretching. This unique feature of the model enables its use for finer regional scale simulations without increasing the number of grid points. The Indian summer monsoon is the strongest component of the global monsoon system and monsoon circulations are important to the Indian and surrounding region because they provide a significant fraction of seasonal rainfall. Much of the Indian Ocean is characterized by a lack of in situ measurements; thus, numerical models rely on remote sensing data and prior forecasts to generate an analysis over this region. The COSMIC GPSRO measurements provide globally distributed atmospheric refractivity soundings including over the Indian Ocean. The GPSRO measurements have relatively high vertical resolution compare to satellite radiances in the lower troposphere and are not contaminated by clouds or precipitation. Hence, This study will explore the improvement in ISM simulation using assimilating GPSRO data on top of the observations, which is being used in NCEP/NCAR reanalysis. Two experiments will be performed; the first one is the control experiment where only observations from NCEP/NCAR reanalysis will be assimilated, and the second one is similar to the first experiment, but also GPSRO data are assimilated in LMDZ5-DART system. The results from above experiments will be presented at the conference.

Keywords: Data Assimilation, COSMIC GPSRO, Indian summer Monsoon

## Projective analysis of staple food crop productivity in adaptation to future climate change in China

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Climate change continually affects our capabilities to feed the increasing population. Rising temperatures have the potential to shorten the crop growth duration and therefore reduce crop yields. In past decades, China has successfully improved crop cultivars to stabilize, and even lengthen, the crop growth duration to make use of increasing heat resources. However, because of the complex cropping systems in the different regions of China, the possibility and the effectiveness of regulating crop growth duration to reduce the negative impacts of future climate change remain questionable. Here, we performed a projective analysis of the staple food crop productivity in double-rice, wheat-rice, wheat-maize and single rice and maize cropping systems in China using modeling approaches. The results indicated that from the present to the 2040s, the warming climate would shorten the growth duration of the current rice, wheat and maize cultivars by 2–24 days, 11–13 days and 9–29 days, respectively. The most significant shortening of the crop growth duration would be in northeast China, where single rice and maize cropping dominate the croplands. The shortened crop growth duration would consequently reduce crop productivity. The most significant decreases would be 27%–31%, 6%–20%, 7%–22% for the late crop in the double rice rotation, wheat in the winter wheat rice rotation and single maize, respectively. However, our projection analysis also showed that the negative effects of the warming climate could be compensated for by stabilizing the growth duration of the crops via improvement in crop cultivars. In this case, the productivity of rice, wheat and maize in the 2040s would increase by 4%–16%, 31%–38%, 11%–12%, respectively. Our modeling results implied that the possibility of securing future food production exists by adopting proper adaptation options in China.

Keywords: model projection, climate change, crop productivity, adaptation

## Optimization of non-ideal parameters of amphibole solid solution using exchange Monte Carlo Method

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Minerals in rocks possess huge information on dynamics of the Earth's interiors within their chemical compositions and textures. Recent progress of analytical instruments and computation abilities enable us to open new approaches to extract information from rocks by machine-learning techniques. In this study, we show the results of petrological optimizing problem by using exchange Monte Carlo method (Hukushima and Nemoto, 1996; Okamoto et al., 2015).

Estimates of P-T paths of metamorphic rocks are of special importance for understanding dynamic behaviors of subduction zones and crusts. Based on Gibbs' phase rule, when the number of compositional variables of a mineral is larger than the degree of thermodynamic freedom of the system, we can obtain pressure and temperature solely from chemical composition of the mineral; this approach is called as Gibbs' method (Spear 1993). Amphibole is one of the most suitable minerals for this analyses, because (1) amphibole is common in various metamorphic rocks, and (2) it has the complex compositions which compositional variables can compensate the degree of freedom, and (3) it commonly show a growth zoning, which is useful for drawing continuous P-T path during its growth. Okamoto and Toriumi (2001; 2004) applied this method to mineral assemblage of amphibole-plagioclase-epidote-chlorite-water in eight component system, in which thermodynamic freedom,  $f$ , is four. By using amphibole compositions, which is written as solid solution of six or seven components, they succeeded in decompression P-T paths from zoning of amphiboles in the Sanbagawa belt.

One of large problems on this thermodynamic analysis using amphibole is the lack of accurate activity model of amphibole due to its complex compositions. Even when we assume simple regular solution model (symmetrical), 21 non-ideal parameters (Margules parameters) are required for mixing of seven endmembers. In binary solution, the Margules parameter is the critical temperature of the solvus, but it is difficult to obtain solvus temperature accurately from complex solid solution like amphibole. Alternatively, Okamoto and Toriumi (2004) proposed the other approach for determining the Margules parameters by using the framework of Gibbs' method as follows. Since the system described above (thermodynamic freedom = 4, independent amphibole component = 5; one amphibole composition is excess), we can estimate one compositional variable of amphibole itself as well as P, T and the composition of other minerals. Accordingly, we can compare the calculated and observed compositions. Using various amphibole compositions from natural metamorphic rocks, we can optimize the Margules parameters from numerous natural data. However, this optimization problem on such many parameters (21  $W$ 's) would have several local minimums or broad minimum, and the results would be sensitive to the analytical errors of amphibole compositions. To overcome this hardly-relaxing problem, in this study, we construct the optimization scheme by using the exchange Monte Carlo Method (Hukushima and Nemoto, 1996). We succeeded the performance of the algorithm by using the synthetic data. We will discuss the applications to natural system and seek appropriate ways to obtain the realistic P-T paths from zoned minerals.

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Keywords: amphibole solid solution, activity model, exchange Monte Carlo method

## Statistical approach in the microboudin method for palaeostress analysis: reliability of the relationship between far-field differential stress and proportion of microboudinage structure of columnar grains

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The microboudinage structure of columnar mineral grains can be used as a passive marker in the palaeostress analysis of the metamorphic tectonites. In this presentation, we demonstrate the stress estimation by the numerical model that uses grain-shape data to calculate the relationship between the proportion of microboudinaged columnar grains ( $p$ ) and the far-field differential stress ( $\sigma_0$ ). This model combines weakest link theory and the shear-lag model. Weakest link theory is used to derive the fracture strength of grains, whereas the shear-lag model is used to determine the relationship between the differential stress within a grain ( $\sigma$ ) and  $\sigma_0$ . An intact grain becomes a microboudinaged grain when  $\sigma$  is higher than its fracture strength at a specific point within the grain. The relationship between  $p$  and  $\sigma_0$  can be used to estimate the magnitude of differential stress. Here, we make calculations of  $p$  for all intact grains under increasing  $\sigma_0$  regarding 50–1000 tourmaline grains shape data. These data are randomly collected from the original 1432 tourmaline grains shape data. Using the calculation result, we enable to evaluate the number of measurement grain to carry out a reasonable palaeostress analysis. This procedure will contribute to resolve the particularly time consuming when conducting stress analysis for a large number of samples within a metamorphic belt.

Keywords: palaeostress analysis, numerical simulation, microboudin palaeopiezometer, tourmaline, microboudinage structure