GeoΣim

4th Annual GeoSim Workshop
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at

GFZ
Helmholtz Centre
POTSDAM

HELMHOLTZ
ASSOCIATION

Contents

Workshop Program

Part I - Morning

Time	Event
10:00 - 10:30	**Registration incl. poster mounting** (coffee available)
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11:00 - 11:20	Johannes Wagner: *Mg2SiO4 forsterite grain boundary structures and self-diffusion from classical molecular dynamics simulations*
11:20 - 11:40	Christopher Irrgang: *Ensemble simulations of the oceanic induced magnetic field*
11:40 - 12:00	**Coffee Break**
12:00 - 12:20	Edoardo Mazza: *Characterization of the meteorological environment associated with the tropical transition of a medicane in the Western Mediterranean.*
12:20 - 12:40	Weishi Wang: *Modelling of the Bank Filtration during Pumping in Nedlitz Potsdam*
12:40 - 13:00	GeoSim - Practical Information Round by Dr. Karen Leever
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Part II - Afternoon

Time	**Event**
14:00 - 14:20	Anthony Osei Tutu: *Effect of plate boundary friction viscosity and upper mantle heterogeneities on global plate velocities geoid and dynamic topography*
14:20 - 14:40	Jorge Bernales: *Lessons from calibrating a numerical ice-sheet model*
14:40 - 15:00	Ariane Papke: *Multiscale structure of atmospheric vortices*
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15:30 - 17:00	Poster Session (coffee and cake available)
17:00 - ??:??	**Social Event** - **optional** Join us at Hafthorn: Friedrich-Ebert-Strasse 90, 14467 Potsdam (http://www.hafthorn.de)

Abstacts by Last Name

Lessons from calibrating a numerical ice-sheet model

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Many crucial physical processes in ice-sheet modeling are accounted for using empirical laws containing uncertain free parameters. These include among others mechanical properties of the underlying bedrock in case of sliding evolution of ice viscosity and ocean-induced melting at the coastal margins which are processes that are often impossible to quantify on a continental scale using direct observations. For the Antarctic ice-sheet our experiments have shown that it is often difficult to obtain a parameter set that produces reasonable agreement between observations and model results. This could be due to limitations in the assumptions underpinning the parametrizations (e.g. the use of constant homogeneous single-value parameters) deficiencies in external forcing and intrinsic limitations in the model. We have tested this hypothesis implementing a simple iterative inverse technique that produces a first-order approximation of the distribution of parameter values required by the model to minimize the deviations from observations. Potential counteracting errors are accounted for performing sensitivity analyzes whereas the uncertainties in the external forcing are explored using several different data sets. Our results suggest that existing parametrizations are often too simple to yield realistic results with parameter distributions that would require improved treatments of the corresponding processes in order to be reproduced. Although simple and by no means definite the method provides valuable insights into the applicability of the simplifying assumptions within the model highlighting those that need to be improved to enable realistic modeling of present-day ice-sheets. We suggest that these conclusions are applicable to many modeling studies where confirming that the model is capable at all of yielding realistic results is a crucial initial step.

Modelling the transport of Carbo-Iron colloids in porous media

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In-situ remediation of groundwater contamination has always been challenging due to restricted access natural heterogeneity and long times scales. The new remediation method is injecting particles that sub-surface and there using their chemical potential to transform contaminants into less harmful substances. However limited mobility fast aggregation and sedimentation of the injected particles are common properties that limit the capability and success of in-situ contaminant remediation. Carbo-Iron Colloids (CIC) is a recently developed type of nano-iron containing particles which consists of activated carbon particles (d50 = 0.8 μm) that are plated with nanoscale zero-valent iron (nZVI) clusters for in-situ transformation of chlorinated solvents. It combines the mobility of activated carbon and the reactivity of nZVI. The objective of the research is to investigate and quantify the mobility of CIC in porous media. In this research simulation using MNM1D (Micro and Nanoparticle transport model in porous media in 1D geometry) are compared with the results from column experiments performed earlier (Busch et al. 2014). The first results depict similarities between the breakthrough curve obtained from the column experiments and simulations. In one example there is a slight shift between the initial part of the curve before it starts reaching the plateau. This might be due to the dead volume in the column which reduces the pulse duration creating this shift of ca. 0.5 pore volumes. Comparing the simulated breakthrough of different underlying kinetics i.e. 1) Linear 2) Blocking 3) Ripening and 4) Straining; the behaviour of the curve is matching better in case of Straining compared to the other three kinetics. Furthermore the colloid transport module of the software HYDRUS which has different formulation of attachment kinetics and 2D and 3D capabilities. It will be further used to compare the breakthrough curve and then also results from a 2D laboratory transport experiment (Busch et al. 2014) and further experiments to be performed with the same physical model 2D aquifer. Using the simulation tools of column and 2D; we expect to acquire deeper understanding of the true kinetics involved in the colloidal transport in the tested porous media. One challenge will be to address the influence of hydro-chemical conditions e.g. pH ionic strength in the simulations. Key words: In-situ remediation colloid transport activated carbon nanoscale zero-valent iron dechlorination Micro and Nanoparticle transport.
Reference: J. Busch T. Meißner A. Potthoff & S.E. Oswald (2014): Investigations on mobility of carbon colloid supported nanoscale zero-valent iron (nZVI) in a column experiment and a laboratory 2D-aquifer test system. Environmental Science & Pollution Research. (21): 10908-10916

A preliminary coseismic rupture model for the Illapel earthquake

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On September 16, 2015, the convergent Chilean margin experienced another huge subduction megathrust earthquake. The Mw =8.3 Illapel earthquake occurred in the central part of Chile and is linked to the eastward subduction of the Nazca plate underneath the South American plate. Combining InSAR data of the new Sentinel satellite mission and GPS displacement measurements, we derive a first preliminary coseismic rupture model for the Illapel earthquake. The rupture nucleated near the coast, close to the city of Illapel but propagated updip to the north. Ground deformation geometry is approximately circular shaped with a diameter of about 100km centered in the middle of the forearc and a peak slip of about 7m. Almost all seismotectonic segments at the highly active plate boundary of South America broke within the last decades. Last huge megathrust events at the Chilean margin took place to the south respectively north of Illapel, in Maule, 2010 (Mw =8.8) and Pisagua, 2014 (Mw =8.2) . The Illapel region itself was last hit by an earthquake with comparable along-strike extent in 1943. Accumulated slip deficit and approximate matching of peak slip defines the Illapel area as a candidate for generating characteristic earthquakes with short recurrence times, especially because the 1943 event was preceded by another event with similar rupture mechanisms in 1880. The degree of locking is generally very high in this area along the coast and the hypocenter is characterized by a local peak in coupling. Partially interseismic creeping is supposed to be taking place to the south of the main rupture. To the north, locking is more gradually decreasing and most likely the rupture terminated against a zone of reduced locking. The Illapel earthquake could relieve much of the accumulated stress in the seismotectonic segment. But the level of observational attention remains high, since the segment to the north of the Illapel area was last ruptured in 1922.

Ensemble simulations of the oceanic induced magnetic field

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The oceanic induced magnetic field has the potential to be utilized as indirect observations of the general ocean circulation. The modelling of this magnetic field is affected by various uncertainties that originate from errors in the input data and from the applied model itself. The amount of aggregated uncertainties and their effect on the modelling of electromagnetic induction in the ocean is unknown. For many applications however the knowledge of model uncertainties is essential. To investigate the uncertainty in the modelling of motional induction simulation experiments are performed on the basis of different error scenarios. This ensemble-based approach allows to estimate both the spatial distribution and temporal variation of the uncertainty in the oceanic induced magnetic field. The largest uncertainty in the motionally induced magnetic field occurs in the area of the Antarctic Circumpolar Current. Local maxima reach values of up to 0.7 nano Tesla (nT). The estimated global annual mean uncertainty in the motionally induced magnetic field ranges from 0.1 to 0.4 nT. Compared to the strength of anomalies of the motionally induced magnetic field the relative amount of uncertainty reaches up to 30 %. The largest relative uncertainty occurs on the northern hemisphere. The major source of uncertainty is found to be introduced by wind stress from the atmospheric forcing of the ocean model. In addition the temporal evolution of the uncertainty in the motionally induced magnetic field shows distinct seasonal variations. Specific regions are identified which are robust with respect to the introduced uncertainties.

Revisiting visco-elastic effects on interseismic deformation and locking degree: a case study of the Peru-North Chile subduction zone

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Viscoelastic effects potentially play an important role during all phases of the earthquake cycle in subduction zones. However most current models neglect such effects in the interseismic deformation pattern. Here we use finite element method (FEM) models to investigate the control of viscoelasticity on interseismic deformation and to highlight the pitfalls of interpreting the data with purely elastic models for both the forward and inverse problems. Our results confirm that elastic models are prone to overestimating the interseismic locking depth a crucial parameter for estimating the maximum possible earthquake magnitude. The application of the viscoelastic model improves the fit to the interseismic deformation especially in the inland area. Additionally we construct 3-D FEM models constrained by geophysical and GPS data and apply our methodology to the Peru-North Chile subduction zone. Our results indicate that viscoelastic effects contribute significantly to the observed GPS data. The signals interpreted as back-arc shortening in the elastic model can be alternatively explained by viscoelastic deformation which in turn dramatically refines the interseismic locking pattern in both dip and strike directions. Our viscoelastic locking map exhibits excellent correlation with the slip distributions

of previous earthquakes especially the recent 2014 Mw 8.1 Iquique earthquake. The incorrect elastic assumptions affect the analysis of interseismic deformation with respect to slip deficit calculations. Our results thus suggest that it is necessary to thoroughly reevaluate existing locking models that are based on purely elastic models some of which attribute viscoelastic deformation to different sources such as microplate sliver motions.

Using Artificial intelligence methods to estimate Air Temperature from MODIS Land Surface temperature over Berlin

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Land Surface Temperature (LST) is defined as the temperature of the interface between the Earth's surface and its atmosphere and thus it is a critical variable to understand land-atmosphere interactions and a key parameter in meteorological and hydrological studies which is involved in energy fluxes. Air temperature is one of the most important input variables in different spatially distributed hydrological ecological and human-biometerorological models. The estimation of near surface air temperature (Ta) is useful for a wide range of applications such as agriculture climate related diseases and climate change studies. Some applications e.g. from traffic or energy management require air temperature data in high spatial and temporal resolution at two meters height above the ground (T2m) sometimes in near-real-time. Thus a parameterization based on boundary layer physical principles was developed that determines the air temperature from remote sensing data (MODIS data aboard Terra and Aqua satellites). Air temperature is commonly obtained from synoptic measurements in weather stations. However the derivation of near surface air temperature (Ta) from the land surface temperature (LST) derived from satellite is far from straight forward. T2m is not driven directly by the sun but indirectly by LST thus T2m can be parameterized from the LST and other variables such as Albedo NDVI Water vapor Building's fraction sky view factor and etc.. Most of the previous studies have focused on estimating Ta based on simple statistical approaches advanced statistical approaches Temperature-Vegetation index (TVX) approach and energy-balance approaches but the main objective of this research is to explore the relationships between Air temperature (AT) and land surface temperature (LST) in Berlin by using Artificial intelligence method with the aim of studying key variables to allow us establishing suitable techniques to obtain Air Temperature from satellite Products and ground data. Secondly to investigate the influence and contribution of each variable on air temperature changes during day and nighttime. In the other hand in this work an attempt was explored to identify an individual mix of attributes that reveals a particular pattern to better understanding variation of air temperature during day and nighttime over the different area of Berlin. Our goal is to identify the patterns that exist among the attributes and to quantify the contribution and influence of each attribute. For this reason a three layer Feedforward neural networks is considered with Levenberg-Marquardt algorithm and with different number of neuron in Hidden layer and different independent variables. Considering the different relationships between air temperature and land surface temperature for different land types enable us to improve better parameterization for LST and air temperature for determination of the best non-linear relation between Land surface temperature and air temperature over Berlin during day and nighttime. The results of the study will be presented and discussed Keywords: Land surface temperature Air temperature MODIS Artificial Neural Network remote sensing.

Correlation Based Geomagnetic Field Modeling

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We present a new method for determining geomagnetic field models. Our approach is purely based on the correlation structure of the geomagnetic field and its observables. Therefore we consider the magnetic potential as a Gaussian random field. An a priori correlation structure is derived from knowledge of the characteristic length scales shapes and distinct sources of the geomagnetic field. As a consequence of that approach measurements are correlated random variables. We use Bayes' theorem which allows to infer for the field's PDF and its a posteriori correlation structure. Furthermore we present a technique which allows for statistically separating various field contributions and an assessment of uncertainties.

Characterization of the meteorological environment associated with the tropical transition of a medicane in the Western Mediterranean

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In order to explain the rare occurrence of medicanes it is necessary to achieve a better understanding of the dynamic and thermodynamic characteristics of the meteorological environment in which they develop. The tropical transition of a medicane in the Western Mediterranean on October 7th 1996 is analyzed by means of COSMO-CLM limited-area ensembles of atmospheric simulations. Cyclone-centred composites of the 27 medicanes and the 23 non-transitioning storms reveal that non-negligible baroclinicity influences the cyclogenesis. As the storms undergo a warm seclusion-like evolution the vertical tilt possessed at early stages is drastically reduced. Significant differences emerge from the composites comparison. Despite the stronger vertical wind shear associated with the transitioning cyclones tropical transition occurs within generally accepted wind shear thresholds. Sensible and latent heat fluxes differences only become positive in the medicane composite after the transition consistent with a modulation of medicanes' intensification rather than formation by the air-sea interaction feedback. Additionally medicanes feature enhanced convection in conjunction with significantly larger divergence aloft and a moister middle troposphere although the environment's potential instability is larger only below 900 hPa. The relative humidity anomaly is largest between 600-700 hPa underneath the greatest differences in vertical velocity and diabatic heating rate. The outcomes point towards an important role of mid-tropospheric moisture in supporting deep convection and promoting enhanced latent heat release by condensation.

Testing a Cross-scale Model of Seismic Cycle

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We model seismic cycle of great megathrust earthquakes using finite element numerical technique that employ elasto-visco-plastic rheology consistent with laboratory data of crustal and mantle rocks and is capable to describe both geological and seismic-cycle time-scale deformation of lithosphere. Here we present details of model design and testing. We prepare model setup by modeling subduction process for several million years with the different assumptions for initial lithospheric structure and temperature of the overriding and subducting plates and kinematic boundary conditions. As a result we get the subduction model with appropriate

geometry and stress distribution. We then substitute static friction by rate and state friction law and employ adaptive time-step integration procedure that changes time step from 40 seconds at instability (earthquake) and gradually increase it to 5 years during postseismic relaxation. We study sensitivity of model in 2D to the magnitude of static friction rate and state parameters (a b and Lcr) and viscosity in subduction channel and demonstrate agreement with theoretical expectations and observations. In particular we obtain almost linear relation between the earthquake period and stress drop from one hand and the rate and state parameter (b-a) from another and realistic values of stress drop of few MPa for the typical great earthquakes. The model also shows classic instable behavior at low Lcr and conditionally stable behavior at high Lcr. Next we investigate dependency of seismic moment (and average slip) of model earthquake on rupture area in 3D. We obtain relations close to the theoretical expectation for the average stress drop of earthquake weakly dependent from its magnitude.

Effect of plate boundary friction viscosity and upper mantle heterogeneities on global plate velocities geoid and dynamic topography

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Plate tectonics and mantle convection are the principal mechanisms controlling the thermal and geological evolution of the Earth. These processes are central to our understanding of the tectonic deformation and thermal and compositional state of the Earth. The driving and resisting forces concentrated at plate boundaries are the results of the current plate motion which is observed. Model predictions of plate velocities their magnitude and pattern depends sensitively on a number of parameters that define the upper mantle viscosity structure plate boundary friction mantle buoyancy etc. Using a finite element code (SLIM3D Popov and Sobolev 2010) coupled with a spectral mantle code (Hager and O'Connel 1981) at the 300 km depth we have calculated plate velocities goied and topography for two different model setups. Firstly we investigate the sensitivity of modeled plate velocities to the choice of viscosity and friction necessary for plate formation. We use the viscosity range $10^{22.5}$ Pa.s to $10^{25.3}$ Pa.s for the lithosphere and $10^{19.0}$ Pa.s to $10^{22.0}$ Pa.s for the asthenosphere while varying plate boundary friction (coefficient) within the range of 0.01 to 0.05. For each individual parameter combination we then estimate the misfit with the observed plate velocities (NUVAL 1A and GPS velocities). Secondly after the incorporation of strong slabs temperature-dependent viscosity and realistic treatment of plate margins in the upper mantle we repeat the same exercise to separate the impact of slab pull which was omitted in the first exercise. Here we used two thermal lithosphere models (Artemieva 2001; Steinberger et al., in review) to include of slabs in the subduction zones and cratonic roots over continental areas. In the first model setup a simplified upper mantle model with asthenosphere depths of 100 km 150 km and 200 km has been used. The optimal coupling between the lithosphere and asthenosphere has been achieved using the asthenosphere viscosity of $10^{20.3}$ Pa.s asthenosphere depthof 200 km and friction coefficient at the plate boundaries of 0.02 resulting in the rms of 3.2 cm/yr. By introducing temperature dependent viscosity and slabs in the upper mantle the coupling between the lithosphere and asthenosphere has been achieved at a mean depth of 110 km with the rms of 3.4 cm/yr. We further calculate the resulting geoid lithosphere boundary stress and topography for each setup and match with observations.

Multiscale structure of atmospheric vortices

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We present a model to study intense vortical flows in the atmosphere with a focus on the spin-up from a tropical storm to hurricane strength. Paeschke et al. (2012) developed a theory describing a new mechanism for the transfer of convectively available potential energy (CAPE) to the primary vortex circulation that involves an interplay of strong vortex tilt with non-axisymmetric patterns of the release of CAPE or of other diabatic heating effects. Strong vortex tilt during early stages of hurricane development is corroborated by observational data presented by Dunkerton et al. (2009). The theoretical hypotheses of Paeschke et al. (2012) is tested against numerical simulations reproducing certain "precessing quasi-modes" of vortices with large tilt in three-dimensional numerical simulations of adiabatic flows. Such quasi-modes which are at the core of the hypothesized spin-up mechanism have been theoretically predicted in a linearized small-displacement theory by Reasor et al. (2004) and a large-tilt analogue has been identified in the nonlinear matched asymptotic analysis of Paeschke et al. (2012).

Addressing structural uncertainty in hydrological modelling: Multiple hypotheses framework and the human factor

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To simulate hydrological processes for a catchment of interest a large number of model hypotheses has been developed. This is primarily the result of insufficient process understanding at the catchment scale which led to a vast number of conceptualisations and (semi-)empirical approaches. A hydrological computer model typically consists one specific formulation and parameterisation of each simulated process called a 'model hypothesis'. The choice for a hypothesis is thereby based on the objective of the study the temporal and spatial scale that shall be covered data availability and environmental characteristics. However there is a high degree of subjectivity and ambiguity during model structure selection implementation and parameterisation herein termed the 'human factor'. The goal of this study is to investigate the uncertainty range from different model hypotheses that are considered to be equally likely representations of relevant processes explicitly including the human factor. The ECo-Hydrological Simulation Environment (ECHSE) is a framework for user-friendly development of eco-hydrological model engines. It further includes a toolbox of process representations which can easily be extended. Using such a framework rather than employing multiple individual models as has been done in several other studies ensures a consistent data handling and avoids side-effects from individual model pre-processing steps. Within the framework several equally likely hypotheses shall be employed and tested. To address the human factor during hypothesis building process representations of the same process are copied from another model and compared to implementations in the simulation environment that have been prepared separately. Furthermore different parameterisations independently compiled by different persons from the same data source are tested. Although it is practically impossible to estimate the complete range of uncertainty this approach gives a rough estimate of two sources of errors structural uncertainty and the human factor that are commonly acknowledged but not addressed explicitly.

Intensity-Duration Relation in the Bartlett-Lewis Rectangular Pulse Model

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For several hydrological modelling tasks precipitation time series with a high (sub-daily) resolution are indispensable. This data is however not always available and thus replaced by model data. A canonical class of stochastic models for sub-daily precipitation is the class of Poisson cluster processes e.g. the Bartlett-Lewis rectangular pulse model (BLRPM). The BLRPM has been shown to be able to well reproduce certain characteristics found in observations. Our focus is on intensity-duration relationship which are of particular importance in the context of hydrological modelling. We analyse several high resolution precipitation time series (5min) from Berlin and derive empirical intensity-duration relations for several return levels of intensities (intensity-duration-frequency curves IDF curves). In a second step we investigate to what extend the variants of a BLRPM are able to reproduce these relations (i.e. the IDF curves) for different situations (e.g. seasons) and for the various return-levels of intensities. By means of a sensitivity study with the BLRPM we investigate to what extend the ability to reproduce the intensity-duration relationships is related to certain relations between the model parameters. Such relations are typically useful to reduce the complexity of the model and thus robustify and facilitate parameter estimation.

Scaling the Sand Box - Mechanical (Dis-) Similarities of Granular Materials and Brittle Rock

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Analogue sand box models are an important tool to understand tectonic deformation. Combining their high spatio-temporal resolution with measurements of boundary forces has recently emerged as a promising approach to comprehend the interplay between deformation and the evolution of transient mechanical parameters. However for the findings of such studies to be representative of natural prototypes the models need to be properly scaled. The common scaling approach does not include any transient behaviour and might thus be too simple. We present here an extensive dataset characterising the mechanical behaviour of a common analogue material and use literature data on natural rock to explore the similarities and dissimilarities between those datasets and to define the limitations of the analogue modelling approach.

FEM for viscoelastic mantle simulation

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Due to the impossibility of direct observations of the actual processes in the earth's mantle numerical simulation plays an important role in advancing their understanding. Furthermore the effects of those processes on and their interaction with the lithosphere/asthenosphere shall be taken into account to verify them. In the past the earth's mantle has been mainly treated as a purely viscous fluid which is not able to resolve the elastic behavior of the mantle due to high stresses. Nowadays a viscoelastic fluid is often used instead to account for it. While the numerical methods and analysis of the Boussineq type equations for viscous mantle flow are well known only few is known about the ones for viscoelastic fluids. Existence and uniqueness results are only available for special rather restricted models. Moreover the numerical solution of these equations is very challenging as they are of mixed type (elliptic/hyperbolic) and thus standard discretization like the standard Galerkin method are not appropriate. However there is the possibility to reformulate the equations to obtain an explicitly elliptic momentum equation. In this special case as well theoretical results as numerical methods are at hand for the steady flow regime. This approach will be followed and hopefully adapted to the non-isothermal flow considered in mantle convection simulation.

Seismotectonic analog models: Materials and scaling

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Analog and numerical models that simulate seismotectonic deformation are normally limited to a small scale-range. This is because of the large range in scales. Typical velocities encompass more than 13 orders of magnitude from km/s (rupture velocity) to mm/a (e.g. tectonic uplift). Numerical models need to encompass this using adaptive time-stepping algorithms. For analog models this is not possible because the models are conducted in real-time. Using stick-slip materials combined with an elastic component it is very easy to produce a complete earthquake cycle. The major problem is the scaling from model time to natural time. Following previous studies we use a dynamic time scale that distinguishes between coseismic and interseismic time. Dimensionless parameters that characterize the processes and materials are used for scaling depending on the state of the model. For example during a seismic event inertia plays an important role and therefore the set of scaling variables is different from the interseismic time. We are establishing an analog model setup to investigate seismotectonic deformation including short-term and long-term effects. The model features a multi-layer lithosphere analog composed of different elastic and viscoelastic materials. To be able to scale our models we have been characterizing a wide range of materials over a broad experimental range. A comparison with natural systems shows that highly concentrated ballistic gelatin combined with viscoelastic silicone oils is suitable to model the behavior of a natural lithosphere. Tectonic background strain scaled to model dimensions is imposed on a precut fault surface in the gelatin. The coated fault surface can produce periodic slip events that are denoted as analog earthquakes. The underlying silicone oil exhibits a Maxwell type postseismic response because of its viscoelasticity. The model is monitored with a 500 Hz and 50 Hz particle image velocimetry camera system. This enables us to trace μm-sized displacements of the faults to estimate the coseismic slip distance. Furthermore stress drops are measured with a dynamometer and the stress field in the model is visualized using photoelasticity.

Hitting Times in Network Analysis

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The structure of networks has been studied using among others spectral methods and average hitting times of a random walker process defined on the vertex set [1 2]. The latter approach has some favourable properties with regards to computational efficiency and allows for an adoption to more general problems. Both in discrete and continuous time settings expected hitting times can be computed conveniently as a solution of a system of linear equations [3]. Many applications yield networks that are immensely big yet sparse to some extent. For the resulting sparse transition matrices hitting times can be computed efficiently whereas eigenvalue decompositions can become almost infeasible. So far spectral approaches have been used mostly for undirected networks where random walker processes are reversible by construction and the spectra of transition matrices contain real eigenvalues only. In that case clusters can be identified as regions on which the dominant eigenvectors are almost constant. It was recently shown that this correspondence can not be extended to general graphs and how to interpret eigenvectors associated to complex eigenvalues remains blurry. As it turns out it is no coincidence that for undirected networks results of approaches based on hitting times often yield results identical to those of spectral methods. A strong point of the former in network analysis is their greater generality being applicable to directed and undirected networks alike while taking the asymmetric nature of directed networks into account.

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How strong might future Grand Minimum simulations be influenced by the choice of the spectral dataset? An Evaluation with a state-of-the-art Chemistry-Climate Model of highest complexity

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The long-lasting minimum of Solar Cycle 23 as well as the overall weak maximum of Solar Cycle 24 reveal the possibility for a return to Grand Solar Minimum conditions within the next decades. The past 1 000 years feature at least 5 excursions (lasting 60 – 100 years) of exceptionally low solar activity induced by a weak magnetic field of the Sun. The last Grand Solar Minima (the Maunder Minimum 1645 - 1715) coincides with the Little Ice Age in Europe a time of severe cold and hardship. The quantification of the implications of such a projected decrease in solar forcing is of ultimate importance given the on-going public discussion of the role of carbon dioxide emissions for global warming and the possible role a cooling due to decreasing solar activity could be ascribed to. However existing model simulations that aim to answer these questions suffer from simplifications in the included parameterizations (e.g. no spectral radiation scheme) missing coupling with ocean models or too low model tops. Besides that there is still no clear consensus about the actual strength of the Maunder Minimum what is reflected in a wide range of spectral reconstruction datasets available. To estimate the range of climate response to different Maunder Minimum reconstructions we tested 3 different solar datasets that show significant differences in both total solar irradiance (TSI) and spectral irradiance (SSI) with a single model first-time. For our purposes we choose to use the ECHAM/MESSy Atmospheric Chemistry Model (EMAC) coupled to a mixed-layer ocean. EMAC incorporates interactive ozone chemistry a high-resolution shortwave radiation scheme as well as a high model top (0.01 hPa). To get a clean climate signal all simulations were conducted in time slice mode under 1960 conditions. The experiments show distinct differences in near surface temperatures and reveal the important role of stratospheric processes for such kind of simulations.

Linking Subduction Seismic Cycle and offshore Morphology along the Chilean margin

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Morphological features at subduction zones are undoubtedly influenced by the complex interplay between the subducting slab and the overriding plate. Several studies suggest that the subduction dynamics is strongly dependent on the geometry and rheology of the margin (including gravity anomalies viscous mantle flows and roughness of the slab among others). However it is not clear how the geomorphological variation along strike can be used as a proxy for better understanding the location and periodicity of large earthquakes and the transfer of stresses among adjacent segments. Here we investigate the links between the kinematics of the interface and the morphology of the overriding plate along the Chilean margin by combining a morphometrical analysis and kinematic numerical models. We constructed swath profiles and subtracted the averaged topography as well as gradient analysis to characterize variations of morphological features. On the coastal area the bathymetry and topography analysis shows a planar feature gently dipping ocean-wards and backed by a cliff which exhibits spatial variations in its width hight and extension along-strike. This morphology suggests a quiescence process or a "stable tectonic condition" at least since the late Quaternary (over multiple seismic cycles) which can be related to the locked zone on the interface and ruptures of great earthquakes. In order to test this hypothesis we built a synthetic 3D finite element model to explore the parameters which might control the extent of this pattern. Doing so we varied the size of the locked zone and the rheology of the overriding plate testing different viscosities and crustal heterogeneities. After simulating several continues seismic cycles the results indicate that this planar feature spatially correlates with the rupture size of recent great earthquakes and locking degree corroborating that the earthquake cycle deformation has an imprint on the offshore morphology.

Mg_2SiO_4 forsterite grain boundary structures and self-diffusion from classical molecular dynamics simulations

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It is well understood that grain boundaries influence many key physicochemical properties of crystalline materials and earth materials are no exception to this. Grain boundaries in the mineral olivine have reshaped our understanding of geophysical processes in the earth's mantle, e.g. in form of enhanced element transport through grain boundary diffusion. Investigations of the relation between transport rate, energy and geometry of individual grain boundaries is compulsory to understand transport in aggregates with a lattice preferred orientation (LPO) that favours the presence and or alignment of specific grain boundaries over random grain boundaries in an undeformed rock. In this contribution, we perform classical molecular dynamics simulations of a series of symmetric and one asymmetric tilt grain boundaries of Mg_2SiO_4 (forsterite), ranging from 9.58° to 90° in misorientation and varying surface termination (see 1). Our emphasis lies on unravelling structural characteristics of high and low angle grain boundaries and how these influence grain boundary energy and self-diffusion processes. To obtain diffusion rates for different grain boundary geometries, we equilibrate the respective grain boundary systems at ambient pressure and temperatures from 1900-2200K and trace their evolution for run durations of more than100 ps. Subsequently, we track the mean square displacement of the different atomic species within the grain boundary layer over time to estimate self-diffusion constants for each grain boundary geometry and temperature. First results suggest that diffusion rates decrease with increasing grain boundary energy. We will discuss these results in the light of recent experimental data and show strength and limitations of the method applied.

1. Adjaoud, O., Marquardt, K., Jahn, S., Phys Chem Miner 39, 749-760 (2012)

Modelling of the Bank Filtration during Pumping in Nedlitz, Potsdam

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Bank infiltration is of great importance for drinking water supply in Europe while the water quality is strongly improved during transportation from the surface to groundwater system. Since the lack of intuitive grasp for the groundwater flow field difficulties for a deep understanding of the underlined theory in this natural phenomenon is increased. To improve the comprehension numerical simulation is introduced as a tool to study the spatial patterns and flow field while its performance is always limited by the calibration accuracy uncertainty of geological structures and the lack of observation values. In some cases calibrated different parameter sets could reach equally accurate result which makes the clarification of the flow field more difficult. In this research the modelling area situates at Nedlitz Potsdam Germany where locates a bank filtration oriented water plant near a newly engineered channel. To begin with a geological model with main focus on the shallow aquifers is set up while the accuracy is seriously influenced by the discontinuous quaternary unconsolidated sediments including glacial tills of different glacier periods and all kinds of sand. Translated into FEFLOW 6.2 a transient groundwater model is set up for both water head and heat simulation. During the calibration it is clearly found that a well calibrated pure hydraulic groundwater model could act poorly for heat transportation which simply means further calibration of heat transportation could be a tool for evaluating model performance and further improve model accuracy.

Maps and Directions

Map of the Telegrafenberg - GFZ Potsdam including Venue House H