A Computer Scientist's Handbook to the Development and Current State of Stress-State Modeling

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Geofluids - *EAS 4190*
4 December 2023
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1. Abstract

The geological sciences has a data problem, but certainly not a lack of it. With millions of sensors live and reporting large volumes of data all the time as well as a many-decades worth of archives, the real question is what to do with it all. For a while, large compilations of empirical measurements and comparisons to broad theoretical models put the calculations in the hands of the geologists. Since only so much can be carried out by hand, this involved numerous heuristical approaches. Gradually, that manual checking made its way into larger database systems and then into the first numerical finite-element models and inverse methods. Since then, computer systems have only grown, allowing for theoretical principles to be tested and constrained. With the growth of remote sensing techniques, computer hardware, and network infrastructure, machine learning has also started to enter into the picture—though many discussions concerning how to formulate the problems and interpret results are still ongoing. This paper seeks to track and define the evolution and trajectory of stress-state modeling as it may be of interest to a Computer Scientist.

2. Introduction

To make sense of recent advancements and where the field is headed, it is necessary to track the evolution of the theory of stress from its classical origins. This paper will first delve into the theory of stress as it is defined mathematically and introduce the requisite vocabulary in Section 3.

3. Mathematical Foundations of Stress

3.1. Stress

In order to understand the dynamics of rocks and fluids in the crust, we must understand what forces are at play. However the notion of force by itself is not really a useful concept in the context of geologic processes because rocks are usually in a quasi-static equilibrium over geological timescales. This means that these forces are typically balanced, making it nearly impossible to measure directly.

Figure 1. Basalt Columns in Garni Gorge, Armenia [11]. The macroscale structure present in these basalt columns provides an example for when the assumptions of the continuum hypothesis may no longer be reasonable.

This quasi-static nature of geological processes is precisely why stress is considered a more appropriate parameter for the study of geodynamics. Stress is the natural result of applying the continuum approximation to rocks. The continuum approximation treats rocks as continuous materials rather than discrete particles. By doing so, it allows geoscientists to describe and model the behavior of rocks at a macroscopic scale, where the effects of individual forces are averaged out. This approximation must sometimes be questioned as rocks may often be sufficiently structured at a large scale, cf. Figure 1.

Stress, often denoted as σ, is defined as the force applied over an infinitesimal area vector, which commonly is given in units of Pa (pascals).

$$\sigma = \lim_{\Delta A \to 0} \frac{\Delta F}{\Delta A} \tag{1}$$

3.2. The Stress Tensor and Principal Stresses

Although there are a sphere of directions which forces can be applied (and a sphere of orientations for the area vector), the resulting stress for an arbitrary orientation can be summarized entirely by a single 3×3 tensor known as the stress tensor. The stress tensor comprises compressional-tensional stresses σ along the diagonal and sheer stresses on the off-diagonal τ. This can be intuited by considering for any orientation, one direction points into the area (i.e. normal to the area) and two directions are orthogonal (i.e. lie in the plane of the area).

$$\sigma = \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} \tag{2}$$

To calculate the stress in any particular direction, $\hat{\mathbf{v}}$, you can project $\hat{\mathbf{v}}$ onto the stress tensor via a simple matrix multiplication. Since $\hat{\mathbf{v}}$ is normalized, the result of the matrix multiplication is identical to a linear transformation on the unit sphere, and hence the set of all these projections constitutes an ellipsoid of stresses.

$$\sigma_{\hat{\mathbf{v}}} = \hat{\mathbf{v}}^{\mathsf{T}} \sigma \hat{\mathbf{v}} \tag{3}$$

Geometrically, one might recall that the ellipsoid has three axes of symmetry—three points on the unit sphere which were scaled up or down but maintained a constant direction throughout the transformation. Indeed, these points are eigenvectors of the stress tensor. The stresses along the principal axes of the ellipsoid are known as the principal stresses, and they are named σ_1, σ_2, and σ_3 such that $\sigma_1 \geq \sigma_2 \geq \sigma_3$. It is worth mentioning that gravity usually generates one of the principal stresses, dubbed the overburden stress σ_V [1].

With respect to the axes of the principal stresses, the stress tensor thus becomes diagonal. This implies that along principal stresses, there is no sheer stress felt by the rock, but all other intermediate directions feel some sheer stress.

$$\sigma = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix} \tag{4}$$

3.3. The Mohr Circle Diagram

We can visualize this via the Mohr circle diagram, which plots compressional stress along the x-axis and sheer stress along the y-axis (Fig. 2). The Mohr circle diagram appears as three semicircles[2] with a shaded region of possible

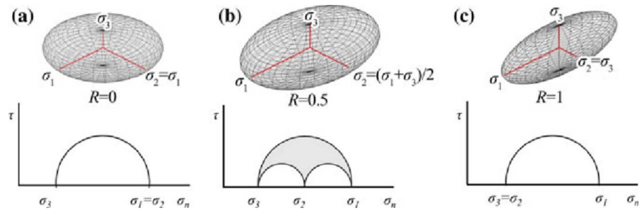

Figure 2. The Stress Ellipsoid (top) and the corresponding Mohr circle diagram (bottom). In (a), the first and second principal stresses have the same magnitude. In (b), the principal stresses are all of different magnitudes. In (c) the second and third principal stresses have the same magnitude. [16]

configurations between them (pictured here in gray). The three points that lie on the stress axis are precisely the three orientations where the stress direction aligns with a principal stress; it is also easy to see that all other orientations must have some sheer component. These semicircles correspond to rotations directly between principal axes and comprise the boundary of the Mohr circle diagram. The large outer circle corresponds to the geodesic on the ellipsoid between σ_1 and σ_3 while the two smaller semicircles correspond to the intermediate transitions σ_1–σ_2 and σ_2–σ_3; all other points are on the interior. Though much more could be said, the ability to represent all possible stress conditions in this manner makes Mohr circle diagrams a frequent and useful tool in understanding geological stresses.

3.4. Further Reading: Measuring Stresses

Stresses tend to be hard to measure. To crudely summarize: it is hard to take measurements inside a rock without modifying the rock in ways which may change the stress-state equilibrium. This is a direct consequence, unfortunately, for relying on the abstraction of continuum mechanics. In order to 'measure' or estimate stress, some other indicator which can be translated from an empirical measurement into the framework of stresses is necessary.

For further information on measurement techniques I recommend (Fairhurst, 2003. cap. 4–11) [12] which gives an overview of various techniques and contextualizes their development. Fairhurst also provides references to the original studies that present the approaches he reviewed.

Because there are so many distinct techniques, for practical considerations about which technique(s) are most appropriate and what can be said about the data gathered from them, (Ljunggren & Chang, 2003) [20] will quite useful.

For a more holistic view of how multiple data sources can be fused, especially as it concerns computational models, see (Stephansson & Zang, 2012. cap. 3) [30].

[1] The overburden stress is due to the weight of the overlying rock; hence for some depth z, $\sigma_V = \int \rho(z) g dz$ where $\rho(z)$ is the density with depth, g is gravitational acceleration, and dz is a depth element.

[2] The Mohr circle diagram is typically shown as a half-space but the full the diagram is mirrored over the compressional stress axis. In its full rendition, the semicircles become circles, but because of this symmetry, typically only the upper half is shown.

4. Numerical Methods

A numerical method is any algorithm which can approximate solutions that cannot be solved for directly. They involve algorithms for computing differential equations and integrals, which are often intractable analytically. In spite of that difficulty, many of these problems are of great interest to us because, to the extent of the model's assumptions, describe fundamental truths about how natural phenomena behave. While many (if not all) of these problems are formulated in terms of differential equations, a review of differential equations is outside the scope of this paper. Instead, I will cover the various categories of numerical methods and explain which problems have been put into terms of those methods.

4.1. Finite Difference Methods (FDMs)

Finite difference methods are perhaps the most straightforward and well-understood algorithms for solving certain differential equations, dating their first use to the time of Euler (Blazek, 2005. cap. 3) [8]. Finite difference methods owe their name to the fact that they discretize space into a lattice of points. The calculus definition of the derivative takes a function and compares it to the value a vanishingly small distance away. In FDMs, this limit is stopped at some finite amount, and hence the name *finite difference*. In particular, instead of taking an infinitesimal step to find the next value of the function, we can take the neighboring element just a short step away.

For implementing a FDM, refer to (Becker & Kaus, 2020. p. 58) [6] for a list of equations known as *stencils*[3] that can be substituted into any FDM with varying results and guarantees. This simplicity of FDMs makes them easy to code but also contributes to their clunkiness in particular settings. Because FDMs require a constant resolution, they make it difficult to probe environments where more detail is required in certain areas than others, or in models which are not easily modeled as a rectangular region. As such, FDMs are often used hybridized with other methods (Carcione, 2022. cap. 9.3.1) [10].

4.1.1 Applications of FDMs

- **Heat Conduction.** Not explicitly related to stresses, but heat transfer is usually a pedagogical starting point, so many resources exist online at a beginner level. FDMs can simulate heat transfer between strata with varying thermal properties (Putra & Fajar & Srigutomo, 2014) [26]. An example implementation in Python (see the FDM notebook) [27].

[3]A 'stencil' is the list of neighbors who are relevant for the approximation at hand. For example, if I need to know the values of my left and right neighbor to calculate the approximation, then my stencil is $[n_{i-1}, n_i, n_{i+1}]$ if I am the i-th node.

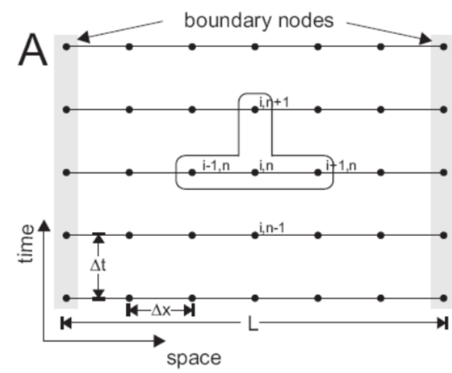

Figure 3. An example of a basic explicit FD stencil (Ruepke, 2021) [27]. In FDMs, both spatial and temporal dimensions have a fixed step size.

- **Stresses.** Due to their stability and predictable error bounds, FDMs make good candidates for balancing stress loads. This is of importance to (Liu et al., 2022) [18] who used FDMs paired with FEMs to model the stress state of low-permeability reservoirs in oil fields. FDMs can also be used to simulate fracture/fault environments where stress becomes heterogeneous, (Sainoki et. al, 2021) [28] demonstrate an approach where faults and fractures are considered as discontinuities and this guides their prediction for stresses in fault damage zones.

- **Wave Propagation.** FDMs have been used to study earthquake mechanics, such as estimating the focal mechanisms[4] at the site of failure and the resulting waveforms. Recent work has applied FDMs to sub-oceanic quakes and how their waves propagate, taking into account interaction between the sea-floor, seawater, and landmasses (Okamoto et al., 2017) [25]. Though FDMs are not known for their speed, modern GPUs allow these simulations to get quite large. There are various open-source repositories which OpenSWPC (Fortran), FDMAP (Fortran), FD-ACOUSTIC (MATLAB, Python)

- **Groundwater.** Since FDMs are adept at modeling static stress configurations, they can also model how fluids behave inside them as those stresses change; for example, (Ku et al., 2020) [17] used a FDM to model ground water responses in aquifers due to tides.

4.2. Finite Element Methods (FEMs)

Finite Element Methods revolutionized the field of complex systems simulation and analysis. FEM breaks down complex geometries into a graph network (typically a

[4]For a brief introduction to focal mechanisms, see this webpage.

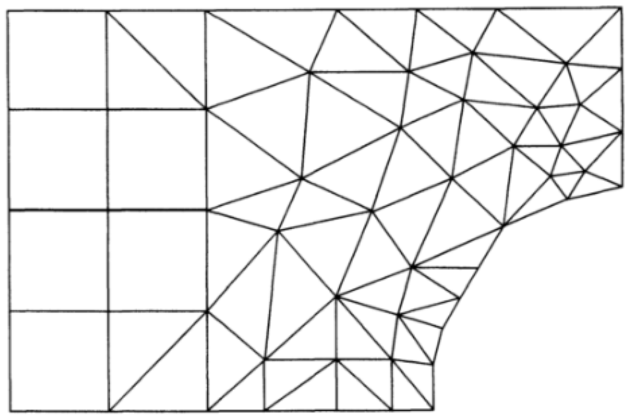

Figure 4. A mesh which demonstrates the kinds of irregular patterns a FEM can solve.

mesh), which allows it to adapt to complex geometries. The method's strength lies in its versatility and precision in handling irregular shapes. Furthermore, FEMs are able to support multi-resolution simulations since nodes can be placed in higher density around regions of importance. Ultimately, FEMs are a superclass of FDMs, so many approaches and formulations discussed earlier can also directly apply to FEMs. Because of their versatility, FEMs are the dominant approach favored across engineering disciplines; most software tools used in engineering analysis, such as those for structural, thermal, and fluid dynamics simulations, incorporate FEM as their core computational technique. This widespread adoption is due to the ability of FEM to accurately model the behavior of materials and systems under various conditions.

The adaptability of FEM to different types of problems is another reason for its popularity. In fact, this cross-collective interest in modeling systems with FEMs has led to bidirectional connectors in order to utilize software between disciplines. One example is Petrel2ANSYS, which is able to take the sophisticated geological models from Petrel and convert them into a format digestible by ANSYS[5] (Liu et al., 2019) [19].

The first step of FEM is the discretization of the domain into a mesh of elements, where each element is typically represented by polynomial shape functions (in FDMs, these are simple linear interpolations). These shape functions are used to approximate the solution within each element. The governing differential equations of the physical problem are then translated into a weak form, often using Galerkin's method. This involves multiplying the PDEs by test functions (which are usually the same as the shape functions) and integrating over the entire domain.

[5] ANSYS is an industry standard for computer aided design in architecture, structural and mechanical engineering, and many other fields.

- **Maximum and Minimum Horizontal Stress.** One thing which appears more common among the FEM methods compared to the FDM methods is the fact that large models of particular regions seem to be nearly exclusively modeled via finite element. Since data acquisition is a process which is often not uniform, using FEMs to provide detail where detail is known can improve simulation accuracy. Take for example (Ziegler et al., 2020) [35], which presents a cumulative model of the stress state of the Bavarian Molasse Basin, estimating values for $S_{H\max}$ and $S_{H\min}$. This was put in context of geothermal projects where it is important to know if the crust is stable or in a critical stress state. Another similar comprehensive model was put together for Germany via the SpannEnD project (Ahlers et al., 2020) [4], which also set out to determine max-min stress directions over the country; later this became a continuous model of contemporary stresses in Germany (Ahlers & Henk et al., 2021) [3].

- **Groundwater.** There has been a wealth of literature on the FEM as applied to groundwater; for classical and theoretical formulations of the problem, (Narasimhan & Witherspoon et al., 1982) [24] is a huge resource. A recent formulation can be found in (Sbai & Larabi, 2023) [29]; they also implement a dynamic meshing algorithm that fits the element boundaries to the phreatic surface, which appears to beat all fixed methods currently published.

- **Faulting and Deformation.** The dynamic boundaries of the FEM can model individual faults; a good example of this is the analysis of fault lines in Southern California performed by (Ye & Liu, 2017) [34]. In an unrelated study on faults in pull-apart basins, (Nabavi et al., 2018) [23] utilized a commercial software package, ABAQUS™. A more recent paper modeling isostacy due to glacial melting benchmarks its approach which uses ASPECT, an open sourced geological solver (which includes Adaptive Mesh Refinement), against ABAQUS™ and TABOO (Weerdesteijn et al., 2023) [32].

4.3. Boundary Element Methods (BEMs)

Boundary Element Methods emerged as a powerful tool for solving boundary value problems. BEM simplifies the problem by focusing on the boundaries rather than the entire domain. By converting volume integrals into surface integrals, it can significantly reduce computational complexity, making it highly efficient for problems involving infinite or semi-infinite domains, such as those encountered in geophysics and acoustics. While not all problems can be formulated in boundary integral form, boundary formulations

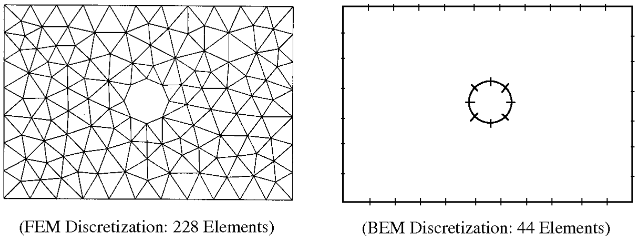

Figure 5. Comparison of a FEM and a BEM for the same space.

are often well suited for problems involving complex geometries and where detailed information is required only on the boundaries. This includes cases where the interior domain less relevant to the problem's focus. For example, in fracture mechanics, the behavior at crack surfaces is critical, while the material's behavior away from the crack is less so. Similarly, in fluid dynamics, the interest might lie in the flow behavior near the boundaries of a vessel rather than the entire fluid volume. Boundary Element Methods offer an efficient approach to these and other similar challenges.

- **Fracture Mechanics.** A review of specific formulations from classical theory is available in (Aliabadi & Brebbia, 1996) [5]; they cover boundary element methods relevant to fracture mechanics. One way of broadening the use-cases of BEMs is to ensemble them with other methods. A more recent approach, UGUCA, is explored in (Kammer et al., 2021) [15]. UGUCA is an open source C++ parallel spectral-boundary-integral method. In their paper they are able to use UGUCA to model dynamic failure surfaces between elastic half-spaces for research in areas like dynamic fracture mechanics, decohesion, and the onset of frictional sliding.

- **Earthquakes.** Recently, more attention has been given towards trying to broaden the problems that BEMs can be applied to. For example (Thompson & Meade, 2023) [31] introduce a new GPU-accelerated method, enabling the efficient solving of problems involving millions of boundary elements. This advancement allows for more realistic and accurate earthquake simulations on complex fault geometries.

- **Wave Propagation.** (Abdullahi et al., 2022) [1] primarily investigate the effects of seismic SH-wave excitation on oil reservoirs using a boundary element method (BEM) in a half-plane model. This study explores how SH-waves, generated through seismic stimulation, impact oil recovery from wells. They used a BEM to model seismic SH-waves from depth through a partially saturated oil reservoir to the ground surface.

5. Learned Methods

Before getting deep into Machine Learning (ML) methods, it is important to take a step back and consider all of what has been said. In every case so far, the approximations and numerical solutions to these problems have been taken from theory along with some simplifying assumptions. In previous sections, we discussed methodologies based on theoretical principles complemented by selected simplifications. These approaches allow for precise error and stability analyses. Machine Learning models, however, are notoriously uninterpretable. ML models operate primarily on the objectives set by the user and the dataset presented to them. The underlying assumptions which these models discover to improve their predictions are not inherently aligned with established physical laws. This shift signifies a notable transition from the more transparent, theory-driven methods to the opaque, data-driven paradigms of ML. Since this is intended for the Computer Scientist, I assume a base understanding of Machine Learning going forth.

5.1. Considerations for Machine Learning

There was a panel held by the AI For Good Discovery series titled "A collective agenda for AI on the Earth sciences" [9] which covers many of ways the field of Earth science is moving forward in light of recent advancements in Machine Learning. With respect to the concerns of interpretability, the first speaker Gustau Camps-Valls, a Professor at the Universitat de València brings to light two important developments with respect to the veracity of model outputs. Firstly, he presents the idea of constrained optimization, which in this context means to instilling some immutable layer at the end of the model which enforces the output. This can take the form of a differential equation, energy conservation, or any other physical fact which the network must not violate. The second aspect involves model interpretability—*how can we extract causal relationships from models?* The answer here is to build in ways of querying the model for causal inference[6].

5.2. Machine Learning for In-Situ Stress

All of the methods described in the following papers share a common theme with respect to Machine Learning in that they apply advanced ML techniques to address complex problems in geosciences and geotechnical engineering. The breadth of techniques is noteworthy, from Random Forest and Adaptive Neuro-Fuzzy Inference Systems to Deep

[6]Professor Camps-Valls goes on to discuss some of his own work on Explicit (Kernelized) Granger Causality, XKGC, giving the example of an atmospheric model predicting that there would be a drought in a particular region. Typically, the model would be completely opaque and the prediction would have to be treated as-is; however, Professor Camps-Valls demonstrates that with XKGC, the parts of the input that the model treats as indicative of this drought are revealed.

U-Net CNN architectures with residuals and the attention mechanism. Most methods have a few things in common: they want to speed up the lengthy computation times from numerical methods or incorporate data priors for ill-posed problems like inverse methods.

1. **Seismic Horizons and Faults.** *"Deep Relative Geologic Time: A Deep Learning Method for Simultaneously Interpreting 3-D Seismic Horizons and Faults"* introduces a deep learning approach to interpret 3-D seismic data (Bi et al., 2021) [7]. It focuses on a volume-to-volume deep neural network, using a U-shaped framework supplemented by multi-scale residual learning and attention mechanisms. The network is designed to segment out relative geologic time (RGT) volumes while simultaneously predicting faults (which look like discontinuities in the RGT). The paper also presents a thorough discussion of its network architecture, custom loss function, data preparation (and augmentation), and even application in various case studies.

2. **Stresses from Logging Data.** In their paper *"Machine learning application to predict in-situ stresses from logging data"* (Ibrahim et al., 2021) [14], the authors aim to predict minimum and maximum horizontal stresses in subsurface formations using well-log data. They train three ML models on different architectures to compare: Random Forest, Functional Network, Adaptive Neuro-Fuzzy Inference System (ANFIS). The results demonstrated the capability of these ML techniques to accurately predict horizontal stresses, with ANFIS slightly winning out. The study highlights the potential of ML to provide an alternative to traditional stress estimation methods.

3. **Beating the Finite Difference Method.** The paper *"A Deep Learning Approach Replacing the Finite Difference Method for In-Situ Stress Prediction"* by (Gao et al., 2020) [13] tests out the possibility of neural networks achieving performance on par with numerical FDM methods. presents a novel deep learning architecture named ES-Caps-FCN, designed to predict in-situ stress in geotechnical engineering. This approach aims to replace the conventional finite difference method (FDM) used for stress prediction (they use FLAC3D as a ground truth). The study demonstrates that their method outperforms traditional methods like linear regression and deep neural networks in terms of accuracy and computational efficiency

4. **Tunnel Deformation.** Another fairly recent paper *"Machine Learning in Conventional Tunnel Deformation in High In Situ Stress Regions"* discusses using machine learning (ML) for predicting tunnel deformation in high-stress geological environments (Ma et al., 2022) [21]. It introduces the MIC-LSTM algorithm, a deep learning method combining the Maximal Information Coefficient (MIC) and Long Short-Term Memory (LSTM) networks. The study covers the challenges in tunnel construction under such conditions, the effectiveness of ML in analyzing various parameters causing tunnel deformation, and provides a comparative analysis with traditional numerical simulation techniques, highlighting the enhanced prediction accuracy of the MIC-LSTM model.

5. **First-Motion Classification.** "CFM: A Convolutional Neural Network for First-Motion Polarity Classification of Seismic Records in Volcanic and Tectonic Areas" introduces a Convolutional Neural Network (CNN) method, called Convolutional First Motion (CFM), to automatically identify first-motion polarities of seismic waves (Messuti et al., 2023) [22]. This deep learning approach is demonstrated to be effective and robust against label noise, achieving high accuracy in classifying seismic waveforms' first-motion polarities. The method's reliability, tested on various datasets, shows great potential for enhancing earthquake and volcanic eruption analysis.

5.3. Future Directions

This is an informal section containing my personal opinions after ingesting many different papers with respect to Machine Learning in the Earth sciences. The backdrop of these opinions is derived from my own work as a computer scientist.

There needs to be a more concerted effort to produce public datasets and benchmarks. In my opinion, it is not fruitful to develop a machine learning method when there are no public datasets with which models can be evaluated over. Machine learning methods are new but they are not so new as to have no precedence in the field—many papers cite previous papers for inspiration on their ML implementations. Even still, few quantitatively compare their implementation with another's (though many papers do compare against their own variants of their own models). Compare this to Computer Vision (CV), for example, where massive datasets like ImageNet, COCO, LAION, CIFAR and PASCAL VOC are perhaps the single most cited papers in all the field. Virtually *all* modern research in Computer Vision is completely dependent on the availability of these datasets and publicly available benchmarks. Admittedly, this effort will be much more difficult in geophysics because the data formats are nowhere near as universal as images and the types of problems are at least as various as the different data formats. There are some open projects which are beginning to tackle this, and I believe the most prominent is

SeisBench (Woollam et al., 2021) [33], which is an open sourced framework for using the latest models, developing datasets, and creating and comparing benchmarks. Ultimately, it does look like things are headed in the right direction. Here's a quote from the paper *"Deep Learning for Seismic Inverse Problems: Toward the Acceleration of Geophysical Analysis Workflows"*:

> "We conclude this article by noting that among the prominent reasons for the outstanding success of DL [Deep Learning] during the past decade is the availability of large-scale open data sets for benchmarking. These data sets enable reproducible research and effective comparisons among different architectures. We anticipate that the future availability of similar data sets for seismic inversion will significantly advance DL solutions in this area" (Adler et al., 2021) [2].

6. Further Reference

While researching, I accumulated this list of interesting items, helpful repositories and codebases which did not fit but still are valuable resources in and of themselves.

1. **Awesome Open Geoscience.** The GitHub repository "awesome-open-geoscience" is a curated collection of open-source resources beneficial for "geoscientists, hackers, and data wranglers". It includes various software tools, data repositories, tutorials, cheat sheets, and other miscellaneous resources. The software tools are categorized into several areas like seismic and seismology, well log, geostatistics, geospatial, geochemistry, geophysics, structural geology, and visualization. This repository is a community effort, open to contributions, and aims to make geoscience-related work more accessible and efficient. For more details, you can visit the repository here.

2. **GeoPlat AI** is a company that centers itself around the enhancement and processing of seismic data. GeoPlat AI is a company specializing in applying machine learning techniques to geophysical data, specifically seismic data, to enhance its resolution and interpretability. (And honestly, they do such a good job that I can hardly believe my eyes—if only they had open research...). Their solutions focus on addressing various challenges in the field of geophysics, such as poor quality or low-resolution seismic data.

3. **MTMOD**, which stands for the Megathrust Modeling Framework, provides a collection of teaching and research software packages and computing environments focused on megathrust earthquakes. Provided tools include calculating seismicity forecasts, coseismic stress and displacement, and earthquake dynamic ruptures. These tools are developed in languages like MATLAB, Python, and Julia, and are available on GitHub. The site also features partner repositories and projects related to earthquakes and seismicity in general.

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