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A Discussion on Geodynamic Modeling Methodology: Inferences from Numerical Models in the Anatolian Plate

Jeodinamik Modelleme Metodolojisi Üzerine Bir Tartışma: Anadolu Levhasındaki Sayısal Modellerden Çıkarımlar

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Abstract: Numerical models have found widespread use in geosciences, mainly due to high-resolution datasets and the development of supercomputing facilities with powerful data processing and storage capabilities during the past two decades. Instantaneous and time-dependent geodynamic modeling studies were carried out in many regions of the Alpine-Himalayan orogenic belt, including the Anatolian Plate, to investigate mantle dynamics such as lower lithosphere deformation, upper mantle flow, and their surface implications.

This study focuses on the instantaneous numerical modeling technique by considering multidimensional thermomechanical models in the Central and East Anatolian plateaus. To this end, conventional geodynamic modeling processes are explained with a conceptual flow chart that shows a feed-forward backpropagation modeling architecture which is nonlinearly fed by a large parameter space. While addressing a complex natural phenomenon controlled by variables on a wide range of space-time scales, the limitations as well as advantages of numerical models are analyzed.

In addition to conventional techniques, systematic data improvement is discussed as a new strategy in data/parameter-dependent numerical model design through an iterative process based on the Grounded Theory method for the construction of an explanatory theory from the model. This involves not refinement but (re)construction of the data (i.e., measurement/analysis/scaling) as an effective way to reveal theory/information grounded in data.

It is speculated that this procedure, which includes problem-oriented data reconstruction accompanying the numerical modeling process, may provide an integrated perspective for instantaneous numerical modelling.

Keywords: Anatolian Plate, geodynamic modeling, geophysics, Grounded Theory, numerical model.

Öz: *Sayısal modeller, son yirmi yılda yüksek çözünürlüklü veri setleri ve güçlü veri işleme ve depolama kapasiteleri olan süper bilgisayar olanakları sayesinde yer bilimlerinde yaygın bir kullanım alanı bulmuştur. Alt litosfer deformasyonu, üst manto akışı ve bunların yüzey etkileri gibi manto dinamiklerini araştırmak için Anadolu Levhası da dahil olmak üzere Alp-Himalaya orojenik kuşağının birçok bölgesinde anlık ve zamana bağlı jeodinamik modelleme çalışmaları yapılmıştır. Bu çalışma, Orta ve Doğu Anadolu platolarında çok boyutlu termomekanik modelleri dikkate alarak, anlık sayısal modelleme tekniğine odaklanmaktadır. Bu amaçla, geleneksel jeodinamik modelleme süreçleri, geniş bir parametre uzayı tarafından doğrusal olmayan bir şekilde beslenen ileri beslemeli geri yayılım modelleme mimarisini gösteren kavramsal bir akış şeması ile açıklanmaktadır. Çok çeşitli uzay-zaman ölçeklerindeki değişkenler tarafından kontrol edilen karmaşık bir doğa olayını ele alırken, sayısal modellerin*

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üstünlüklerinin yanı sıra sınırlamaları da burada analiz edilmektedir. Geleneksel tekniklere ek olarak, sistematik veri iyileştirme, modelden açıklayıcı kuramın oluşturulmasında Temellendirilmiş Kuram yönteminin yinelemeli bir süreci aracılığıyla veri/parametre bağımlı sayısal model tasarımında yeni bir strateji olarak tartışılmaktadır. Bu, verilere dayanan teoriyi/bilgiyi ortaya çıkarmanın etkili bir yolu olarak sadece veri iyileştirmeyi değil, verilerin (yeniden) inşasını (yani ölçüm/analiz/ölçeklendirme gibi) içerir. Sayısal modelleme sürecine eşlik eden problem odaklı veri yeniden yapılandırmasını gösteren bu prosedürün, anlık sayısal modellemeye bütünleşik bir bakış açısı sağlayabileceği düşünülmektedir.

Anahtar Kelimeler: *Anadolu Levhası, jeodinamik modelleme, jeofizik, Temellendirilmiş Kuram, sayısal model.*

INTRODUCTION

Multidimensional instantaneous (time-independent/present-day) and time-dependent (evolution) numerical models are a complex form of scientific hypotheses (Oreskes et al., 1994) that are used to investigate internal planetary forces that consistently affect the Earth’s topography, plate boundaries, crustal and lithospheric deformation processes (e.g., Pysklywec et al., 2000; 2002; Pysklywec and Beaumont, 2004; Ismail-Zadeh and Tackley, 2010; Flament et al., 2013; Faccenna and Becker, 2010; 2020; Gerya, 2022; Davies et al., 2023; Lanari et al., 2023). Numerical models, therefore, help to better understand complex natural processes that can be controlled, for example, by the rheology of materials (and/or viscosity, King, 2016) such as temperature, density, and petrographic properties at a wide range of spatiotemporal scales. Rheology is used here to refer to the flow of materials in liquid and/or solid-state, which indicates viscous behavior rather than elastic deformation in response to applied forces (Ranalli & Murphy, 1987) by analogy with the motto “everything flows (πάντα ῥεῖ)” of Simplicius of Cilicia, an Anatolian philosopher and mathematician (1st century BC, Beris and Giacomin, 2014).

In this paper, the focus is on instantaneous geodynamic models involving a process of theory construction from data to investigate time-independent variations originating in the upper mantle. To this aim, numerical models in the Anatolian Plate are considered (Şengül Uluocak et al., 2016; 2021) with a discussion about the heuristic nature of numerical modeling in geosciences. First, the numerical modeling strategy was analyzed through the conventional modeling approach and then a systematic problem-oriented data reconstruction procedure is discussed as an improvement to the numerical geodynamic modeling design.

INSTANTANEOUS GEODYNAMIC MODELING ARCHITECTURE

Multidimensional thermomechanical models of the Central and East Anatolian plateaus (Şengül Uluocak et al., 2016; 2021), which are discussed here specifically, were conducted following the conceptual flow chart in Figure 1, partly presented for conventional numerical modeling (e.g., Ismail-Zadeh and Tackley, 2010). That is, the model inherently begins with a research problem and continues in turn with the definition of physical and mathematical models, numerical methods and coding, and subsequent construction of explanatory theories. The systematic research process in Figure 1 refers to a feedforward (forward modeling) backpropagation (inversion) modeling architecture where the geodynamic concept determines what type of data will be used in the model and the data (observations and/or laboratory experiments) feeds the model nonlinearly. This approach involves evaluating the results and tuning/adjusting parameters and boundary conditions to avoid oversimplification and/or missing inputs, although some simplifications (e.g., 3-layered earth model, Figure 2a) are inevitable when modeling spatially-temporally constrained 3-dimensional (3D) natural processes.

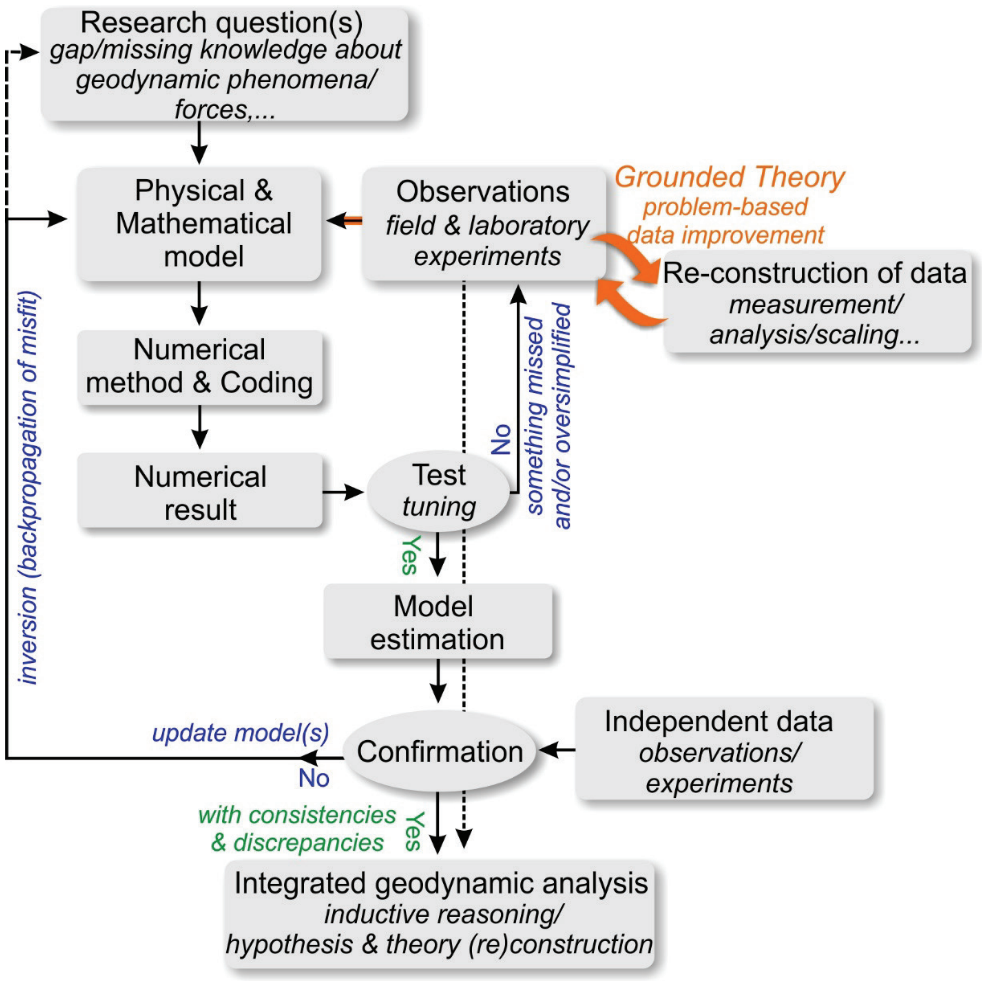

Figure 1. Conceptual flow chart showing feed-forward backpropagation modeling architecture for the instantaneous numerical geodynamic model. Orange arrows indicate the data reconstruction procedure following the Grounded Theory (GT) method.

Şekil 1. *Anlık sayısal jeodinamik model için ileri beslemeli geri yayılımlı modelleme mimarisini gösteren kavramsal akış şeması. Turuncu oklar Temellendirilmiş Teori yöntemini izleyen veri yeniden yapılandırılması sürecine işaret etmektedir.*

Possible mismatches between estimations and multidisciplinary independent datasets are optimized systematically during the inversion procedure using empirical approaches, as well as statistical and probabilistic inversion methods (e.g., Van Zelst et al., 2022 and references therein). This is shown as confirmation in Figure 1, implying the legitimacy of the estimation (e.g., Oreskes et al., 1994). In practice, following visual inspection including pattern recognition and qualitative comparison, the independent variables are iteratively renewed to achieve the most possible unique result (viz. empirically adequate result, e.g., Oreskes et al., 1994 and references therein) that addresses the research problem. For instance, comparing spatial patterns and amplitudes is a common way to analyze the agreement between model results and observations (e.g., Şengül Uluocak et al., 2019; Faccenna and Becker, 2020). Thus, finally, the model provides an ultimate result with insight that enables the modeler to (re)produce and/or to (re)interpret independent observations (e.g., surface heat flow, magmatism, density, crustal and lithospheric boundaries) and relate them to the natural phenomena (e.g., lithospheric removal, crustal extension).

In Central and Eastern Anatolia (Figure 2), numerical models were designed based on material properties derived from numerous observations and laboratory experiments (e.g., Ranalli, 1995; Hirth and Kohlstedt, 1996; 2003; Naliboff and Buiter, 2015; references in Şengül Uluocak et al., 2021) with three compositional layers (i.e. crust, lithospheric mantle, and asthenosphere) extending from the surface to depths of 1000 km (Figure 2b) and 600 km (Figure 2d). Average thicknesses for crustal and lithosphere-asthenosphere (LAB) boundaries (ranging from ~30-43 km for the Moho, ~60-140 km for the LAB, e.g., Şeber et al., 2001; Starostenko et al., 2004; Pamukçu et al., 2007; Zor, 2008; Molinari and Morelli 2011; Priestley et al., 2012; Priestley and McKenzie, 2013; Laske et al., 2013; Kheirkhah et al., 2013; Yegorova et al., 2013; Karabulut et al., 2019) were used (e.g., 36 km and 60 km in Central Anatolia, Figure 2b). Densities were obtained from seismic data (Piromallo and Morelli, 2003) and have good agreement with the latest high-resolution seismic tomography models, especially in terms of large-scale variations of upper mantle structures beneath the Anatolian Plate (e.g., Portner et al., 2018; a compilation of seismic tomography models in Şengül Uluocak et al., 2021). Thermal fields were obtained based on the thermal expansion rule; $\rho(T) = \rho_0 (1-\alpha\Delta T)$, where ρ_0 is the reference density (e.g., Figure 2b) and α is the coefficient of thermal expansivity (K^{-1}). The temperature gradient (ΔT, Figure 2b) with normal geotherms was used to obtain the temperature field (cross-section in Figure 2d, Karato, 1993; Demetrescu and Andreescu, 1994; Shaw and Pysklywec, 2007; Komut et al., 2012; Şengül Uluocak et al., 2016).

In the mathematical model (Figure 1), thermal convection and deformation were calculated for an incompressible medium by using the Boussinesq approximation for the conservation equations of mass (, momentum , and energy , where v is the velocity -m/s; is the stress tensor; is density; g is the gravitational acceleration- m/s^2; C_p is specific heat capacity- J/kg/K; T is the temperature-K; t is time-s and k is thermal conductivity-W/m/K) (e.g., Fullsack, 1995; Bangerth et al., 2019). The stress tensor () changes depending on the plastic yield stress and viscous stress in the calculations () (e.g., Pysklywec et al., 2000; Glerum et al., 2018; Bangerth et al., 2019; Van Zelst et al., 2022 and references therein). The effective viscosity () is a function of the second invariant of the deviatoric strain rate tensor () and temperature , where B is the viscosity parameter ($Pa^{-n}s^{-1}$), n is non-Newtonian viscosity exponent, Q is activation energy ($Jmol^{-1}$) and R is the universal gas constant ($Jmol^{-1}K^{-1}$). The transition zone was defined by considering viscosity variation between the upper and lower mantle in the 2D model (i.e., a 100-fold increase in viscosity at 660 km depth) along the profile A-A' (Figure 2a and 2b). Boundary conditions were set as a free surface on the top allowing for dynamic topography caused by normal fluid stresses in the underlying mantle, and free slip for the rest of the boundaries.

Since the process requires the analysis and calculation of large volumes of data, all models were run on supercomputing clusters using different open-source libraries and numerical modeling codes based on the finite element method (SOPALE and ASPECT, Fullsack, 1995; Pysklywec et al., 2002; Kronbichler et al., 2012; Heister et al., 2017; Bangerth et al., 2019). Time-dependent changes, such as erosion, internal heating and sedimentation, were neglected in the instantaneous models. Estimations were obtained from a series of numerical results testing different parameters (test/tunning) such as densities, thicknesses, strain rates/viscosity, and temperature configurations in the investigated regions. The reader is referred to Şengül Uluocak et al. (2016; 2021) for further details of the initial parameters used in the numerical models.

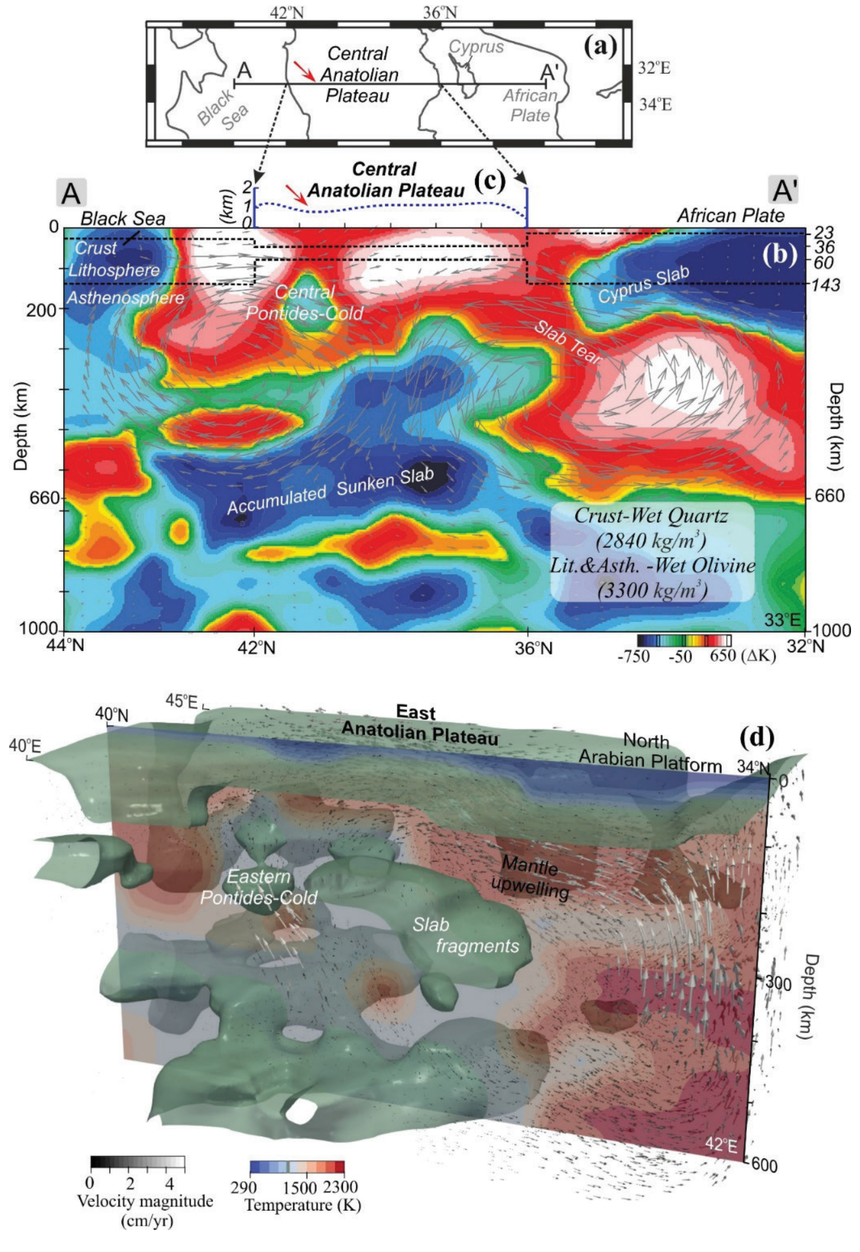

Figure 2. a) Location of Profile A-A' (33°E) in Central Anatolia. **b)** 2D temperature variations with Moho and LAB interfaces (black lines, see text for references). **c)** Dynamic topography along the profile in Central Anatolia. Gray arrows in (b) show the upper mantle-induced convection pattern (modified from Şengül Uluocak et al., 2016). **d)** 3D variation of cold upper mantle structures with mantle flow vectors from the surface to a depth of 600 km. Cross-section of the temperature field (42°E) beneath Eastern Anatolian Plateau (modified from Şengül Uluocak et al., 2021).

Şekil 2. a) *Orta Anadolu, A-A' Profilinin konumu (33°E).* ***b)*** *Moho ve LAB ara yüzleri (siyah çizgiler) ile 2B sıcaklık değişimi (kaynaklar metinde sunulmuştur).* ***c)*** *Orta Anadolu'yu kesen profil boyunca dinamik topografya. (b)'deki gri oklar üst manto tarafından indüklenen konveksiyon modelini/dokusunu göstermektedir (Şengül Uluocak vd., 2016'dan düzenlenmiştir).* ***d)*** *Soğuk üst manto yapıları ve manto akış vektörlerinin yüzeyden 600 km derinliğe değin 3B değişimi. Doğu Anadolu Platosu altındaki sıcaklığın kesiti (42°E) (Şengül Uluocak vd., 2016'dan düzenlenmiştir).*

RESULTS and DISCUSSION

2D and 3D mantle flows are presented with temperature models mainly based on seismically inferred mantle structures beneath the Anatolian Plate (Figure 2). The purpose here is to show variations with a discussion of overall findings and introduce an iterative process of the Grounded Theory method to obtain the most unbiased/unique modeling results. Accordingly, thermomechanical model estimations (Figure 2b-d) indicate long-wavelength (> ~150 km) dynamic support of the observed topography (~ 1 km in Central Anatolia, Figure 2c) in response to the upwelling mantle beneath the plateaus. Along the cross-section (A-A', Figure 2a) cutting across Central Anatolia, the result shows the upper mantle support imaged as northward flows through the Cyprus slab tear in the south of the study area (Figure 2b). Towards the north of the profile, return flows that are bounded by the dense/cold material of the Black Sea region and the northward subducted ruptured-Cyprus slab accumulating in the mantle transition zone are observed (Figure 2b). The 3D model, on the other hand, reveals a significant SW-NE directional mantle flow at long wavelengths with a westward regional flow pattern in the East Anatolian Plateau (Figure 2d). These general findings are in good agreement with numerous observations (e.g., Biryol et al., 2011; Legendre et al., 2021; Şengül Uluocak et al., 2016; 2021 and references therein) and lithospheric removal hypotheses proposed for these parts of the Anatolian Plate. For instance, a lithospheric drip under the Central Anatolian arc/Kırşehir arc (Göğüş et al., 2017) and lithospheric delamination or progressive lithospheric peeling under the East Anatolian crust (Göğüş and Pysklywec, 2008; Memiş et al., 2020) support the idea that the study regions are isostatically uncompensated and significantly affected by an upwelling mantle in concordance with slow upper mantle seismic tomography anomalies (e.g., Portner et al., 2018; Kounoudis et al., 2020; Şengül Uluocak et al., 2016; 2021).

As a result, it can be concluded from the modeling estimations here that multidimensional instantaneous thermomechanical models obtained by the conventional modeling approach provide useful information about the upper mantle-induced forces and their surface effects in the study regions. Yet it should be noted that relative quantitative results may involve some uncertainties/inconsistencies mainly due to the limited knowledge of subsurface structures and poorly constrained data used in the numerical models (e.g., Şengül Uluocak et al., 2019; Petrescu et al., 2023). In this case, a high-resolution physical model with data (such as density, temperature, etc.) sensitive to relatively small-scale structures (e.g., crustal heterogeneities), for instance, could be used to improve numerical results and interpretations. The crust-based model with a viscously strong lithospheric layer beneath the Central Anatolian Plateau, the T-2 model based on the latest regional tomography data in Eastern Anatolia, and the combined temperature model (Model-2) in the Southeast Carpathians are some examples of model improvement applications (Şengül Uluocak et al., 2016; 2019; 2021). Refinements of parameters and thus of results (i.e. inversion in conventional modeling) will not be further elaborated here. From a critical point of view, however, it can be argued that the estimations are often data (and/or parameter)-dependent and that sometimes problem-oriented refinements to the data may be necessary to exploit the heuristic results of the numerical model.

Overall, given that the results of geodynamic models are not unique and their accuracy may not be fully tested, ultimate outcomes exclusively provide an approximation to nature with an argument that needs to be falsified. Unlike the standalone mathematical models and numerical coding of the principals driving the flow in the upper mantle, verification and/or validation of the estimations might be impossible mainly due to geodynamic models with empirically-based input parameters not being closed systems in which all components are correct and founded independently (Oreskes et al., 1994; Chandra et al., 2019). Namely, there is no ultimate model that satisfies all observations and solves the whole conundrum with a complete 3D view of mantle deformation. It should also be noted that a more complex model does not necessarily mean a more reliable/accurate result (e.g., Van Zelst et al., 2022). Contrarily in fact, I suggest that a simple model, with a heuristic nature derived from a wide parameter space, often says more. This is the case especially with the results obtained from the conventional modeling approach that also includes empirical inversion processes as discussed here. The implication is that while addressing a complex research phenomenon by using instantaneous numerical geodynamic models, it is worth considering the discrepancies as well as consistencies between results and independent observations, and/or previous hypotheses. For example, the relationship of the modeling results with relatively small-scale Pontides-cold anomalies and uppermost mantle structures beneath Eastern Anatolia (i.e., slab fragments, Figure 2) does not appear to be consistent with previous hypotheses and/or with some of the regional seismic tomography models (e.g., Şengül Uluocak et al., 2021 and references therein). That is, an active drip-like deformation and/or a piecemeal Tethyan slab foundering are not generally accepted hypotheses to explain the lithospheric removal beneath Central and Eastern Anatolia, respectively. However, model results may lead the interpretation of upper mantle-induced forces, as well as the emergence of new research questions for the detailed study on related anomalies.

Unlike the hypothesis-dependent evolution models (theory-first), instantaneous numerical models (facts-before-theory) are substantially dependent on the resolution and sensitivity of the chosen primary data sets, even if optimization has been made during the inversion stage to achieve possible unique/adequate results. Leaving aside a methodological discussion on what counts as data and the fundamental so-called secure knowledge used to measure/collect it, the *a priori theory* only considered in thermomechanical models is that nature with observable properties can be known using scientific methods without requiring pre-formulated postulates. In other words, the numerical models shown here were designed based on data (observations and laboratory experiments) without any previous theoretical input (e.g., slab tear, lithospheric drip, and delamination, etc.), therefore, information that is embedded in data plays an important role in the results. To extract this information (a theory according to the context here) from data, performing data analysis and also measurements iteratively during the modeling procedure may be suggested as a way to improve data quality/sensitivity and/or problem-oriented data acquisition at scales chosen in the numerical models. These processes shown as orange arrows in Figure 1 indicate not adjustment and/or refinement but the substantial reconstruction of data. Namely, orange arrows imply a relationship between the modeling problematic and the process of data construction (i.e., measurement/analysis/scaling) and show a practical way to improve numerical models using problem-oriented data. Hence, the question of "observations: what for?" (e.g., Şengör, 2019) involves a dynamic process in numerical modeling and is iteratively re-answered by reconstructing the data in each problem.

In this manner, the proposed modeling procedure follows orthodox Grounded Theory (GT), which was first introduced by Glaser and Strauss (1967) for qualitative research in social science as a strategy to construct a theory inductively derived from data. Since then, the GT method has been elaborated further and extended for different quantitative and qualitative research areas (e.g., Strauss & Corbin, 1990; Glaser 1992; Diaz et al., 2023). All in all, as can be inferred from the conventional GT perspective, which shares a 'bottom-up' conception of scientific inquiry with the abductive theory of method (e.g., Magnani et al., 2018 and references therein; Danermark et al., 2019), data used in the instantaneous numerical model should be approached in the most unbiased way possible, with a strategy that involves iteratively reconstructing data (with or without data collection) that should be followed to understand what the data implies. Together, my analyses lead to the conclusion that the modeling approach introduced here could be highly functional for modelers/geoscientists in terms of avoiding data waste for the sake of theory and by eliciting theory grounded in data.

GENİŞLETİLMİŞ ÖZET

Bu çalışmada, yer bilimlerinde karmaşık bir araştırma olgusu ele alınırken kullanılan jeodinamik sayısal modellerin metodolojisi üzerinde bir tartışma yürütülmüştür. Bu amaçla öncelikle, geleneksel sayısal jeodinamik modelleme yöntemi, Anadolu Levhasındaki (Orta ve Doğu Anadolu platoları) güncel (zaman-bağımsız) 2 ve 3-boyutlu termomekanik modellerden (Şengül Uluocak vd., 2016; 2021) yararlanılarak ve Şekil 1'de sunulan kavramsal akış şemasındaki adımlar izlenerek açıklanmıştır. Çalışmada örneklendirilen modellerin sonuçları (Şekil 2) genel olarak değerlendirilmiş, güncel-çok boyutlu sayısal modellerin kısıtlıkları ve üstünlüklerine değinilmiştir. Bu aşamada modellerin doğası gereği elde edilen göreceli değişimler ve dolayısıyla jeodinamik model tasarımında bir iyileştirme stratejisi olarak sayısal modellemede sistematik veri yapılandırması üzerinde durulmuştur. Önerilen bu yaklaşım burada da örneklendirilen ve zaten yapılagelen veri düzeltme/iyileştirme süreçleri yanısıra, sayısal modelleme çalışmalarında kullanılan verinin önemli ölçüde probleme dayalı olarak (yeniden) inşasını içermektedir. Böylelikle, sosyal bilimlerde yaygın olarak kullanılan Temellendirilmiş Kuram yaklaşımının yer bilimlerinde sayısal modelleme stratejisi kapsamındaki kullanımına dikkat çekilerek, hipotez (buradaki kavramsallaştırma doğrultusunda; kuram) uğruna veriyi göz ardı etmekten kaçınmada ve veriye dayalı kuramın ortaya çıkarılmasında Yer Bilimciler/Modelciler için son derece işlevsel olabileceği değerlendirilmiştir.

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