# Numerical modeling of stresses and deformation in Zagros-Iranian plateau region

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## Key Points

• We have computed stresses and deformation of Zagros-Iran region with finite element modeling.

• Lithospheric stresses play an important role in the east of Iran.

The joint models of lithosphere and mantle convection are able to explain various deformation
 indicators in the study area.

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#### Abstract

Zagros orogeny System resulted due to collision of the Arabian plate with the Eurasian plate. The 11 region has the ocean-continent subduction and continent-continent collision; and convergence veloc-12 ity shows variation from east to west. Therefore, this region shows the complex tectonic stress and a 13 wide range of diffuse or localized deformation between both plates. The in-situ stress and GPS data 14 are very limited and sparsely distributed in this region, therefore, we performed a numerical simula-15 tion of the stresses causing deformation in the Zagros-Iran region. The deviatoric stresses resulting 16 from the variations in lithospheric density and thickness; and those from shear tractions at the base 17 of the lithosphere due to mantle convection were computed using thin-sheet approximation. Stresses 18 associated with both sources can explain various surface observations of strain rates,  $S_{Hmax}$ , and 19 plate velocities; thus, Surface observations of strain rates, S<sub>Hmax</sub>, plate velocities etc. are explained 20 using the joint models of lithosphere and mantle, suggesting a good coupling between lithosphere 21 and mantle in most parts of Zagros and Iran. As the magnitude of stresses due to shear tractions 22 from density-driven mantle convection is higher than those from lithospheric density and topogra-23 phy variations in the Zagros-Iranian plateau region, mantle convection appears to be the dominant 24 driver of deformation in this area. However, the deformation in the east of Iran is caused primarily 25 by lithospheric stresses. The plate velocity of the Arabian plate is found to vary along the Zagros belt 26 from north-northeast in the southeast of Zagros to the northwest in the northwestern Zagros, similar 27

- to observed GPS velocity vectorsPlate motion of Arabian plate is found to vary along the Zagros
   belt from north-northeast in south-east of Zagros, north in central Zagros to slight northwest in the
   northwestern Zagros. The output of this study can be used in seismic hazards estimations.
- 31 Keywords- Stress field, Gravitational Potential Energy, Mantle convection, Zagros, collision

## <sup>32</sup> Plain Language Summary

We used numerical models to study the stresses causing deformation in the Zagros-Iran region. The 33 stresses are generated due to variations in the density and topography of the lithosphere, which were 34 computed through Gravitational potential energy (GPE) difference. Mantle convection produces shear 35 tractions that are also an important source of stresses causing deformation. Different models of crustal 36 structure and density of lithosphere give varying GPE, thus leading to different interpretations of the type 37 of deformation in the study area. On the other hand, all mantle convection models in our study predicted 38 consistent deviatoric stresses and were able to explain most observations of  $S_{Hmax}$ , plate velocities, and 39 strain rates. Despite this, the lithosphere plays an important role in driving deformation, especially in 40 the east of Iran. Overall, the lithospheric stresses when combined with those from mantle convection 41 gave the best fit to the observed data. 42

## **1** Introduction

Zagros mountains are a part of the Alpine-Himalayan belts that originated due to the Arabian plate 44 colliding with southern boundary of the Eurasian plate. This collision resulted from thein closing of 45 the Neotethys Ocean and formed Zagros fold and thrust belt (Agard et al., 2005, 2011; Alavi, 1980; 46 Mouthereau et al., 2012). The Zagros mountains extend from the eastern part of the Anatolia for over 47 1500 km in the NW-SE direction till the Makran subduction zone, showing large-scale diffuse deforma-48 tion. Despite the first-order characteristics of Though there has been an increase in the influx of various 49 studies trying to constrain the active deformation and present-day kinematics of Zagros orogen is rela-50 tively well understood (Allen et al., 2011; Le Dortz et al., 2009; Reilinger et al., 2010; Vernant et al., 51 2004; Walker, 2006), there are debates about various processes in this region, e.g. the timing of the colli-52 sion is debated. Various authors (Jolivet & Faccenna, 2000; Agard et al., 2005, 2011; Vincent et al., 2005; Ballato 53 have suggested that collision onset time to be in Late Eocene to Oligocene; however, Timing of collision 54 ranges from Cretaceous (Alavi, 1994; Mohajjel & Fergusson, 2000) to Miocene (Berberian & King, 55 1981) or Eocene (Allen & Armstrong, 2008; Jolivet & Faccenna, 2000). However, there has been an 56 increasing consensus on Late Eocene to Oligocene for the onset of collision (Jolivet & Faccenna, 2000; 57

Agard et al., 2005, 2011; Vincent et al., 2005; Ballato et al., 2011; Mouthereau et al., 2012; Koshnaw 58 et al., 2019). Ghalamghash et al. (2009); Mazhari et al. (2009) have argued Late Palaeocene or Early 59 Eocene for the onset of collision. The Zagros and its foreland area have a great source of natural 60 resources like petroleum. The study area consists of the ocean-continent subduction as well as the 61 continental collisions. The convergence rate of the Arabian plate relative to the Eurasia varies from 62 east to west (Figure 1). These complex structures and convergence velocity variation made the variable 63 tectonic stress and deformation. The geophysical, geological and geodesy studies show that these areas 64 are seismic active based on the earthquake data, fault slip rates and GPS velocities, which is related to 65 the complex stress field in this region The Arabia-Eurasia collision zone is a tectonically active region, 66 where ongoing convergence is accommodated by distributed shortening across the Zagros Mountains 67 and the northern and eastern margins of the Iranian Plateau and the southern Caspian Sea. The rate 68 of convergence of Arabia relative to Eurasia also varies significantly, decreasing from 36 mm/yr in the 69 east to 16 mm/yr in the west (Figure 1). The diverse structures, tectonic history, and convergence ve-70 locity variations in the Zagros-Iran plateau region lead to variable tectonic stresses and deformations, 71 thus making it the focus of various geophysical, geological, and geodesy studies (Engdahl et al., 2006; 72 Hatzfeld et al., 2010; Khorrami et al., 2019; Masson et al., 2006; Tunini et al., 2016, 2017). Based on 73 earthquake focal mechanisms, fault slip, and GPS velocities, the Zagros-Iran region has been catego-74 rized as a highly seismic region; thus a better constraint on stresses and deformation in this region may 75 be helpful in disaster mitigation studies. 76

Generally, tectonic stress refers to the forces acting on the Earth's crust that cause it to deform or un-77 dergo changes and it's classified by the first, second and third order on the spatial scale (Heidbach et al., 78 2007; Zoback, 1992). The first-order stresses originate due to the plate boundaries force like ridge push, 79 slab pull and continental collisional; and second-order stresses by the rifting, isostasy and deglaciation. 80 Moreover, third-order stresses are caused by local sources like interaction faults systems, topography and 81 density heterogeneity. Therefore, to understand the origin of these stresses, in-situ stress measurements 82 are done using the focal mechanism inversion, wellbore breakouts, hydraulic fracturing and overcoring, 83 and compiled under the word stress map project. However, in-situ stress data are sparsely distributed and 84 limited, so numerical modeling plays an important role in understanding the kinematics and dynamics of 85 the Zagros-Iran region. Numerical modeling of tectonic stresses and deformation is generally conducted 86 in two approaches (1) using 2D and 3D geometrical structure, plate boundary forces like ridge push, slab 87 pull and continents collision forces and rheological properties like Young's modulus, Poisson's ratio, vis-88 cosity, density etc. (Coblentz & Sandiford, 1994; Dyksterhuis & Müller, 2008; Koptev & Ershov, 2010; 89 Richardson et al., 1976; Yadav & Tiwari, 2018), and, (2) considering Gravitational Potential energy and 90 shear tractions from mantle convection with thin sheet approximation (Bird, 1998; Flesch et al., 2001; 91

<sup>92</sup> Ghosh & Holt, 2012; Lithgow-Bertelloni & Guynn, 2004; Singh & Ghosh, 2020). Therefore, the world
<sup>93</sup> stress map (WSM) provides in-situ stress measurement and the compilation from the focal mechanism,
<sup>94</sup> hydrofracturing, and borehole breakout. However, the in-situ stress (WSM) and GPS velocity data
<sup>95</sup> (ArRajehi et al., 2010; Bayer et al., 2006; Frohling & Szeliga, 2016; Khorrami et al., 2019; Masson et al., 2006, 24
<sup>96</sup> are very limited and sparsely distributed in this region; therefore, there is need for a numerical simulation
<sup>97</sup> study to comprehend the knowledge.

Although numerical modeling of tectonic stress and deformation was conducted in two approaches 98 (1) using 2D and 3D geometrical structure, plate boundary forces like ridge push, slab pull and continents 99 collision forces and rheological properties like Young's modulus, Poisson's ratio, viscosity, density 100 (Dyksterhuis & Müller, 2008; Coblentz et al., 1994; Koptev & Ershov, 2010; Richardson et al., 1976; Yadav & Ti 101 and, (2) considering Gravitational Potential energy and shear tractions from mantle convection with thin 102 sheet approximation (Bird, 1998; Lithgow-Bertelloni & Guynn, 2004; Flesch et al., 2001; Ghosh & Holt, 2012; Si 103 Stress studies showed that it's classified by the first, second and third order on the spatial scale (Zoback, 1992; Heidt 104 The first-order stresses are originated due to the plate boundaries force like ridge push, slab pull and 105 continental collisional; and second order stress by the rifting, isostasy and deglaciation. Moreover, 106 third-order stress are caused by local sources like interaction faults systems, topography and density 107 heterogeneity. 108

There are various studies that have tried to investigate present-day stresses and deformations of the 109 Zagros-Iranian plateau region using focal mechanism inversions, GPS data and numerical modeling. 110 The stresses were computed through the inversion of focal mechanisms in areas like the Zagros fold-111 and-thrust belt (Nouri et al., 2023; Sarkarinejad et al., 2018; Yaghoubi et al., 2021), Zagros-Makran 112 transition zone (Ghorbani Rostam et al., 2018), western Zagros (Navabpour et al., 2008), NW Iran-113 SE Turkey (Mokhoori et al., 2021), NE Lut Block, Eastern Iran (Rashidi et al., 2022; Raeesi et al., 114 2017), and the south Caspian (Jackson et al., 2002). The GPS studies also provide constraints on 115 the present-day deformation in Zagros-Makran transition zone (Bayer et al., 2006), Makran subduc-116 tion zone (Frohling & Szeliga, 2016), Iran (Khorrami et al., 2019; Masson et al., 2006, 2007; Ver-117 nant et al., 2004; Walpersdorf et al., 2014), Nubia-Arabia-Eurasia plate system (Reilinger & Mc-118 Clusky, 2011).numerical studies conducted for tectonic stresses and deformation in Zagro-Iranian region 119 (Austermann & Iaffaldano, 2013; Md & Ryuichi, 2010; Franccois et al., 2014; Khodaverdian et al., 2015; Vernant 120 Sobouti & Arkani-Hamed (1996) studied the large scale tectonic processes of the region and repro-121 duced observed faulting patterns by considering highly rigid central Iran and the South Caspian Sea 122 using a viscous thin-sheet approximation. On the other hand, Md & Ryuichi (2010) used finite ele-123 ment modeling (FEM) to analyse the neotectonic stress field of Zagros and adjoining area modelled 124 the maximum horizontal compressive stress (S<sub>Hmax</sub>) orientations and showed N-S/NNE-SSW oriented 125

S<sub>Hmax</sub> in Lurestan and eastern Zagros Simple Folded Belt, whereas they were aligned in NW-SE directions 126 around Main Recent fault (MRF) and in the northern High Zagros Faults (HZF). Sobouti & Arkani-Hamed (1996) 127 reproduced observed faulting patterns by considering highly rigid central Iran and the South Caspian 128 Sea using a viscous thin-sheet approximation. Further, the kinematic model by Khodaverdian et al. 129 (2015) provided procided constraints on fault slip rates, plate velocities and seismicity of the Iranian 130 Plateau. Most of the deformation studies done in this region focus on different tectonic fragments 131 of the Arabia-Eurasia collision zone. Moreover, the previous studies do not include the role of shear 132 tractions associated with mantle convections in affecting the deformation and stresses in the Zagros-133 Iran regions. The previous models did not include the mantle convections derived shear tractions for 134 computation of deformation and stress in the Zagros-Iran regions. 135

In this study, we investigate the stress and deformation in Zagros-Iranian Plateau region to constrain the forces acting in this region with gravitational potential energy (GPE) and shear traction of mantle tractions. We will use a thin viscous sheet model based on Flesch et al. (2001) to compute various deformation parameters such as deviatoric stresses, strain rates, most compressive principal stress ( $S_{Hmax}$ ), and plate velocities within the Zagros-Iran region.

## **141 2 Tectonic and Geology**

The evolutionrise of the Zagros mountain belt is a direct consequence of continental collision between 142 the Arabian and Eurasian plates. Zagros are located at the northeastern margin of the Arabian plate, 143 trending in the southwest direction (Figure 1). It is bounded by the Main Zagros thrust (MZT) in the 144 northeast, while it joins the Tauras mountains in southern Turkey in the northwest. In the southeast, N-S 145 trending Minab-Zandan fault zone separates Zagros from the Makran range. Outer Zagros are the young 146 folded mountains in the southwest parts of the orogeny (Falcon, 1974; Sattarzadeh et al., 2002). High 147 Zagros fault (HZF) separates highly deformed metamorphic rocks of inner Zagros from Simply folded 148 mountains of outer Zagros (Hatzfeld & Molnar, 2010; Hatzfeld et al., 2010). Inner Zagros are bounded 149 by MZT in the northeast and are dominated by thrust faulting, possibly due to compression during the 150 Late Cretaceous (Alavi, 1980). The northwestern Zagros isare separated from central Zagros by a north-151 south trending strike-slip zone of deformation, known as Kazerun Fault System (KFS) (Authemayou 152 et al., 2005). 153

Zagros mountains were formed between  $\sim$ 35 and  $\sim$ 23 Ma due to the convergence of the Arabian platform beneath the central Iranian crust (Agard et al., 2005; Ballato et al., 2011; Mouthereau et al., 2012). The Arabian plate moves towards Eurasia with a plate velocity of 22-35 mm/yr (DeMets et al., 1990; McClusky et al., 2000; Jackson et al., 2002; McQuarrie et al., 2003; Reilinger et al., 2006) in

N-S to NNE direction. Zagros mountain belt is also accompanied by The convergence of two rigid 158 plates of Arabia and Eurasia leads to a zone of widespread deformation in the form of the high plateaus 159 of Iran. Iranian plateau extends from the Caspian Sea and the Kopeh Dagh range in the north to the 160 Zagros Mountains in the west. Iranian plateau is bounded by the Persian Gulf and Hormuz Strait in 161 the south and the political borders of the country on the eastern side. Several tectonic processes such 162 as intracontinental collisions, subduction along the Makran and the transition from Zagros fold-thrust 163 belt to the Makran subduction zone contribute to the complex tectonics of the Iranian plateau. Numerous 164 earthquakes occur in these high terrains due to sustained tectonic activities; hence, these areas are prone 165 to large seismic hazards. 166

During the last few decades, various geophysical studiessurveys (receiver functions, deep seismic, 167 GPS and tomographic) studies) have been carried out in the Zagros-Iran region to investigate the struc-168 ture and deformation in this region. The southeastern Zagros accommodate the convergence between 169 Arabia and Eurasia by pure shortening occurring through high-angle  $(30^{\circ} - 60^{\circ})$  reverse faults that are 170 perpendicular to the belt (Hessami et al., 2006; Irandoust et al., 2022; Walpersdorf et al., 2006). On 171 the other hand, oblique convergence in central and northern Zagros is partitioned into a strike-slip com-172 ponent that is accommodated on MRF and shortening occurring across the belt (Jackson et al., 2002; 173 Talebian & Jackson, 2002). Zagros is separated from Makran subduction zone (MSZ) by Minab-Zendan-174 Palami (MZP) fault ( $54^{\circ} - 58^{\circ}E$ ), which is a right-lateral strike-slip fault (Bayer et al., 2006). East of 175 MZP shows significant shortening that is accommodated through the subduction in MSZ. Due to the 176 difference between convergence rates, a shearing occurs in eastern Iran which is accommodated by the 177 N-S trending faults bounding the Lut block. In northern Iran, fold and thrust belt of Alborz accommo-178 dates a quarter of the Arabia-Eurasia convergence Irandoust et al. (2022). The oblique convergence in 179 eastern Alborz is also partitioned into shortening at the southern boundary and a left-lateral component 180 across the mountain belt (Irandoust et al., 2022; Khorrami et al., 2019; Tatar & Hatzfeld, 2009). Alborz 181 mountains extend into Talesh in the west which shows thrust faulting on nearly flat faults. Kopeh-Dagh 182 range in northeast accommodates the Arabia-Eurasia convergence through N-S shortening on major 183 thrust faults in the south. 184

## 185 **3** Modeling

### 186 3.1 Equations

<sup>187</sup> To model the present-day stresses causing deformation in the Zagros-Iranian plateau due to the Arabia-<sup>188</sup> Eurasia collision, we solve <del>three-dimensional (3D)</del> the force balance equations, considering the thin 189 sheet approximation.

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$$\frac{\partial \sigma_{ij}}{\partial x_i} + \rho g_i = 0 \tag{1}$$

<sup>191</sup> Here  $\sigma_{ij}$ ,  $x_j$ ,  $\rho$ , and  $g_i$  indicate the  $ij^{th}$  component of the total stress tensor,  $j^{th}$  coordinate axis, density <sup>192</sup> and acceleration due to gravity respectively (England & Molnar, 1997; Ghosh et al., 2013b).

In the above equation, total stress,  $\sigma_{ij}$  is substituted by deviatoric stress using the following relation:

$$\mathbf{\tau}_{ij} = \mathbf{\sigma}_{ij} - \frac{1}{3}\mathbf{\sigma}_{kk}\mathbf{\delta}_{ij} \tag{2}$$

<sup>195</sup> In the above equation, the Kronecker delta and mean stress are denoted by  $\delta_{ij}$  and  $\frac{1}{3}\sigma_{kk}$  respectively. The <sup>196</sup> force balance equation (1) is integrated up to the base of lithospheric sheet (L), resulting in following <sup>197</sup> full horizontal force balance equations:

$$\frac{\partial \overline{\tau}_{xx}}{\partial x} - \frac{\partial \overline{\tau}_{zz}}{\partial x} + \frac{\partial \overline{\tau}_{xy}}{\partial y} = -\frac{\partial \overline{\sigma}_{zz}}{\partial x} + \tau_{xz}(L)$$
(3)

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$$\frac{\partial \overline{\tau}_{yx}}{\partial x} + \frac{\partial \overline{\tau}_{yy}}{\partial y} - \frac{\partial \overline{\tau}_{zz}}{\partial y} = -\frac{\partial \overline{\sigma}_{zz}}{\partial y} + \tau_{yz}(L)$$
(4)

In equation (3) and (4), the over bars indicate integration over depth. Both equations (3 and 4) contain the first term representing horizontal gradients of GPE per unit area inon the right hand side. On the other hand, the shear tractions at the lithosphere base (*L*) arising due to mantle convection are denoted by  $\tau_{xz}(L)$  and  $\tau_{yz}(L)$  (Ghosh et al., 2009).

Both of the force balance equations (3 & 4) were solved using the finite element technique (Flesch et al., 2001; Ghosh et al., 2009, 2013b; Singh & Ghosh, 2019, 2020) for a 100 km thick lithosphere of varying strength (Figure S1a). The laterally varying viscosities for the lithosphere were assigned from Singh & Ghosh (2020). After solving these equations, we obtained the horizontal deviatoric stresses,  $S_{Hmax}$ , strain rates as well as plate velocities and compared them with observations.

<sup>209</sup> The quantitative comparison between predicted and observed  $S_{Hmax}$  axes (Figure 3a) was performed <sup>210</sup> by computing the misfit given by  $sin\theta(1+R)$  (Ghosh et al., 2013a; Singh & Ghosh, 2019, 2020), where <sup>211</sup> R represents the quantitative difference between stress regimes of observed and predicted  $S_{Hmax}$ , while <sup>212</sup>  $\theta$  denotes the angular difference between both. Hence, this misfit accounts for both the angular and <sup>213</sup> regime misfits with values lying between 0 and 3.

The correlation between predicted deviatoric stresses and GSRM strain rates (Figure 3b) (Flesch et al., 2007; Ghosh et al., 2013b; Singh & Ghosh, 2019, 2020) is given by following equation:

$$-1 \leq \sum_{areas} (\varepsilon.\tau) \Delta S / \left( \sqrt{\sum_{areas} (E^2) \Delta S} * \sqrt{\sum_{areas} (T^2) \Delta S} \right) \leq 1$$
(5)

where  $E = \sqrt{\dot{\epsilon}_{\phi\phi}^2 + \dot{\epsilon}_{\theta\theta}^2 + \dot{\epsilon}_{\phi\theta}^2 + \dot{\epsilon}_{\theta\phi}^2 + \dot{\epsilon}_{\theta\phi}^2} = \sqrt{2\dot{\epsilon}_{\phi\phi}^2 + 2\dot{\epsilon}_{\phi\phi}\dot{\epsilon}_{\theta\theta} + 2\dot{\epsilon}_{\theta\theta}^2 + 2\dot{\epsilon}_{\phi\theta}^2}, T = \sqrt{\tau_{\phi\phi}^2 + \tau_{\theta\theta}^2 + \tau_{\phi\theta}^2 + \tau_{\phi\theta$ 217  $= \sqrt{2\tau_{\phi\phi}^2 + 2\tau_{\phi\phi}\tau_{\theta\theta} + 2\tau_{\theta\theta}^2 + 2\tau_{\phi\theta}^2}, \text{ and } \epsilon.\tau = 2\dot{\epsilon}_{\phi\phi}\tau_{\phi\phi} + \dot{\epsilon}_{\phi\phi}\tau_{\theta\theta} + \dot{\epsilon}_{\theta\theta}\tau_{\phi\phi} + 2\dot{\epsilon}_{\theta\theta}\tau_{\theta\theta} + 2\dot{\epsilon}_{\phi\theta}\tau_{\phi\theta}}.$  In the above 218 equation, the second invariants of the strain rate and stress tensors are denoted by E and T. GSRM strain 219 rates, area and predicted deviatoric stresses are represented by  $\dot{\epsilon}_{ij}$ ,  $\Delta S$ , and  $\tau_{ij}$  respectively. To constrain 220 the plate velocities, we compute RMS as well as angular misfit between observed and predicted plate 221 velocities. We also get the relative plate velocities and strain rates as output from models. However, to 222 calculate the absolute plate velocities and strain rates, we require absolute viscosity values. We compute 223 the scaling factor for relative viscosities by placing the predicted velocities in a no-net-rotation (NNR) 224 frame, such that  $\int (v \times r) dS = 0$  and minimizing the misfit between the predicted dynamic velocities and 225 those from Kreemer et al. (2014). Here v denotes the horizontal surface velocity at position r and S is 226 the area over the Earth's surface (see Ghosh et al. (2013b) for details). 227

#### 228 **3.2** Crustal Models

In the right hand side of equations (3 & 4), the first term represents the vertically integrated vertical stress. It is computed and integrated from the top of variable topography up to depth L (100 km) (England & Molnar, 1997; Flesch et al., 2001; Ghosh et al., 2013b; Singh & Ghosh, 2019, 2020) using the following relation:

$$\overline{\sigma}_{zz} = -\int_{-h}^{L} \left[ \int_{-h}^{z} \rho(z') g dz' \right] dz = -\int_{-h}^{L} (L-z) \rho(z) g dz \tag{6}$$

where  $\rho(z)$ , *L* and *h* denote density, the depth to the lithosphere base (100 km) and topographic elevation respectively. *z* & *z'* are variables of integration and *g* represents the acceleration due to gravity. We also calculated the stresses for thicker lithosphere (L=150 km and L=200 km) as studies have shown a much thicker lithosphere in the region (Robert et al., 2017; Tunini et al., 2017) (Figure S2).

The right hand side of equation 6 is given by the negative of GPE per unit area. To calculate GPE 238 and the stresses associated with it, we used three global crustal models, CRUST2.0 (Bassin et al., 2000), 239 CRUST1.0 (Laske et al., 2013), and LITHO1.0 (Pasyanos et al., 2014). The upper crust thickness lies 240 within 15-20 km in the Zagros-Iran region for CRUST2 model (Figure 2a). However, the thickness of the 241 upper crust in the Zagros-Iranian region is much higher for CRUST1 and LITHO1 (> 25 km) (Figures 242 2b & c). The Zagros-Iran region has a thicker middle crust (> 20 km) in the case of both CRUST2 and 243 LITHO1 models (Figures 2d & f), while CRUST1 shows a much thinner middle crust (< 12 km) in this 244 region (Figure 2e). The lower crust in the Zagros-Iran region is found to be very thin (< 10 km) for all 245 three models (Figure 2g-i). 246

<sup>247</sup> The density variations in the study area are minimal for CRUST2 model. CRUST2 also shows

the highest average density in all three layers (>2.7  $g/cm^3$ ) (Figure 2j,m,p). CRUST1 also indicates 248 an average density of  $\sim 2.72 \ g/cm^3$  in the Zagros-Iran region for the upper crust (Figure 2k). The 249 middle and lower crustal layers of CRUST1 show average densities of 2.80  $g/cm^3$  and  $\sim 2.85 g/cm^3$ , 250 respectively (Figure 2n,q). LITHO1 model shows the lowest average density in the study area for all 251 three layers (Figure 21,0,r). The upper crust of LITHO models shows an average density of  $\sim 2.65$ 252  $g/cm^3$ . Central Iran block has relatively denser upper crust (~2.75  $g/cm^3$ ), while the density decreases 253 to  $\sim 2.62-2.64 \ g/cm^3$  near the Zagros region. Similar patterns of density variations are observed in the 254 middle and lower crust of LITHO1 model ((Figure 20,r). Such differences in thickness and density data 255 lead to varying GPE values, and hence subsequently, different stresses. 256

#### **3.3** Mantle Convection

We ran mantle convection models using HC (Hager & O'Connell, 1981). HC is a semi-analytical mantle 258 convection code that uses density anomalies derived from seismic tomography models and radial vis-259 cosity as inputs. Here, we considered four global mantle convection models, S40RTS (Ritsema et al., 260 2011), SAW642AN (Mégnin & Romanowicz, 2000), 3D2018\_S40RTS and S2.9\_S362 to infer the man-261 tle density anomalies. 3D2018\_S40RTS is a merged model of SV wave upper mantle tomography model, 262 3D2018\_Sv given by Debayle et al. (2016), and S40RTS. S2.9 is a global tomography model of the up-263 per mantle with higher resolution which is given by Kustowski et al. (2008b). We merged this model 264 with the global shear wave velocity model, S362ANI (Kustowski et al., 2008a) to obtain the merged 265 tomography model of S2.9\_S362. We used two different radial viscosity structures, namely GHW13 266 which is the best viscosity model from Ghosh et al. (2013b), and SH08 given by Steinberger & Holme 267 (2008). GHW13 is a four layered viscosity structure, with a highly viscous lithosphere ( $\sim 10^{23}$  Pa-s). 268 The viscosity drops to  $\sim 10^{20}$  Pa-s in the asthenosphere, which again increases to  $\sim 10^{21}$  Pa-s in upper 269 mantle and  $\sim 10^{22}$  Pa-s in the lower mantle (Figure S1b). On the other hand, the viscosity in SH08 270 model increases gradually with depth and it has a slightly weaker lithosphere as compared to GHW13. 271 It has the highest viscosity value of  $10^{23}$  Pa-s around 2000-2300 km depth, and significantly lower vis-272 cosity for D" layer (Figure S1b). GHW13 viscosity model performed slightly better than SH08 in fitting 273 the observed parameter, thus we have shown results from the same throughout this paper. However, we 274 have also included the the predicted results and their fit to the observables in the supplementary section 275 (Table S1). The radial viscosity model from Ghosh et al. (2013b), was used in our study to run mantle 276 convection models. 277

#### 278 3.4 Data

To have better constraints on <del>our</del> this study's models, we also estimated  $S_{Hmax}$  (most compressive horizontal principal axes) orientations as well as plate velocities. Various deformation indicators such as  $S_{Hmax}$  orientations from the World Stress Map (WSM) (Heidbach et al., 2016), strain rates and plate velocities from Global Strain Rate Model (Kreemer et al., 2014) were used to perform a quantitative comparison with <del>our</del> the predicted results of this study (Figure 3).

WSM data is a global database of the crustal stress field obtained from various sources such as focal 284 mechanisms; geophysical logs of borehole breakouts and drilled induced fractures; engineering methods 285 such as hydraulic fractures and overcoring; and geological indicators that are obtained from fault slip 286 analysis and volcanic alignments. These data have been assigned quality ranks from A to E based on 287 the accuracy range. A-type data suggests that the standard deviations of  $S_{Hmax}$  orientations are within 288  $\pm 15^{\circ}$  range,  $\pm 20^{\circ}$  for B-type,  $\pm 25^{\circ}$  for C-type and  $\pm 40^{\circ}$  for D-type. However, E-type indicates the 289 data records are either incomplete or from non-reliable sources or the accuracy is  $> \pm 40^{\circ}$ . Our This 290 study uses A-C quality stress data records (Figure 3a). Observed S<sub>Hmax</sub> axes are aligned in NNE-SSW 291 directions in Zagros with dominant thrust faulting. NW and Central Iran show some strike-slip mode of 292 deformation with NE-SW compressional directions. 293

The strain rates and plate velocities are taken from GSRM v2.1 model (Kreemer et al., 2014) (Figure 3b). GSRM v2.1 provides a global data set of strain rates and plate motions that are determined using ~ 22,500 geodetic plate velocities. Higher strain rates are observed along the simply folded mountains (~  $40 - 100 \times 10^{-9}/yr$ ). Most of Iran shows strain rates in between  $4 - 10 \times 10^{-9}/yr$ . The plate motions used in our study for comparing with predicted velocities are given in a no-net-rotation (NNR) frame interpolated on a  $1^{\circ} \times 1^{\circ}$  grid. The velocity vectors show an eastward motion in the study area, which becomes nearly E-W in Afghan Block (Figure 3b).

## **301 4 Results**

#### **4.1** Stress and deformation due to GPE

Three crustal models (CRUST1.0, CRUST2.0 and LITHO1.0) were used to compute GPE within the study region. The second invariant of stress computed using GPE lies within  $\sim$ 10-12 MPa along the Zagros for CRUST2 and CRUST1 models (Figure 4a,c). LITHO1 model predicts larger stress magnitudes along Zagros (Figure 4e). NE-SW compressional stresses are observed along the frontal faults of Zagros (MFF) (Figure 1a,c). The central part of Zagros thrust faults (MZT) shows the strike-slip mode of faulting for nearly all three models (Figures 4 & 4b,d & f). The strike-slip regime further extends into Sanandaj-Sirjan Zone (SSZ) while lies north of MZT for CRUST2 and LITHO1 model (Figure
4b,f), while it transitions to thrust type of deformation in the north of MZT for CRUST1 (Figure 4d).
The Urmia-Dokhtar Magmatic Arc (UDMA) and central Iran also show the strike-slip mode of faulting for CRUST2 and LITHO1. The north of MRF shows tension for CRUST2 model, while CRUST1
predicts this area to be predominantly strike-slip. On the other hand, the entire region shows significant
compression for LITHO1 model.

We compared predicted  $S_{Hmax}$  from our three GPE only models to observed  $S_{Hmax}$  orientations and 315 type obtained from WSM (Heidbach et al., 2016) by computing Regime misfit (Figure 5, left panel). 316 The average misfit is lowest for LITHO1 model with a value of 0.59 (Figure 5g), while CRUST2 model 317 shows the highest average misfit of 0.77 (Figure 5a). High misfits (2-3) are observed North of MRF 318 and Tehran for CRUST2, while lowest (< 1) in case of LITHO1, suggesting that the dominant mode 319 of faulting in this area is possibly thrust as opposed to normal deformation predicted by CRUST2. In 320 central Iran,  $S_{Hmax}$  misfit is low (< 1) when the dominant mode of deformation is strike-slip as predicted 321 LITHO1 model. 322

On calculating the correlation between the predicted deviatoric stresses and GSRM strain rates, the 323 LITHO1 model shows the highest average correlation (0.92) (Figure 5, middle panel). The correlation 324 is found to be extremely poor  $(\sim -1)$  for CRUST2 model in the north of MRF (Figure 5b). Such 325 poor correlation suggests that the predicted stresses differ entirely from those causing deformation. For 326 example, anti-correlation in north of MRF suggests that the dominant mode of deformation in this area 327 might be thrust rather than normal faulting. Again, the correlation coefficient is less than 0.2 in the 328 central Iranian Block for CRUST2 and CRUST1 models (Figure 5b,e), while LITHO1 model shows a 329 better correlation suggesting the strike-slip type of deformation to be more prominent in central Iran 330 (Figure 5h). 331

<sup>332</sup> We predicted the plate velocities for all three models in the NNR frame and compared them with <sup>333</sup> observed plate velocities obtained from Kreemer et al. (2014) (Figure 5 right panel). CRUST2 gives <sup>334</sup> the least RMS error (7.32 mm/yr) and the lowest angular misfit ( $5.5^{\circ}$ ) (Figure 5c). LITHO1 model <sup>335</sup> shows high misfits (> 20°) between observed and predicted velocities in the east of the central Iran (i.e. <sup>336</sup> Afghan Block)(Figure 5i). Both CRUST2 and LITHO1 models predict the plate velocities very close to <sup>337</sup> observed ones in the Zagros mountains, as shown by nearly zero angular misfits along Zagros (Figures <sup>338</sup> 5c & i). CRUST1 performs average in predicting the plate velocities in the study area (Figure 5f).

Interestingly, the use of thicker lithosphere to calculate GPE leads to the introduction of more compressional stresses in the region (Figure S2a-f). The average misfit between predicted and observed  $S_{Hmax}$  is found to be lowest for the 200 km thick lithosphere (Table S2). Similarly, the correlation between strain rate tensor and predicted stresses,; and rms error between observed and predicted NNR velocities show significant improvement for thicker lithosphere. However, the improvement in fit is better for CRUST2 as opposed to the other two models, CRUST1 and LITHO1, where the misfit between
observed and predicted velocities show an increase. Thus, we can say that while considering lithospheric
contributions only, the thicker lithosphere does a better job of explaining the observed deformation indicators (Table S2).

#### **4.2** Stress and deformation due to Mantle Convection

The deviatoric stresses predicted using all four mantle convection models are found to be mostly com-349 pressional along MFF (Figure 6). All models, except for SAW642AN, predict the strike-slip mode of 350 faulting in NW parts of Zagros with nearly E-W oriented extensional axes and N-S compressional axes 351 (Figures 6a, e & g). On the other hand, SAW642AN shows predominant compression within this area 352 (Figure 6e). S40RTS, 3D2018\_Sv, and S2.9\_S362 show strike-slip deformation in NW parts of SSZ, 353 UDMA and NW Iran. Central Iran is predicted to have mostly compressional stresses by all models 354 except for S40RTS. Thrust type of deformation is predicted in Afghan Block by all models with some 355 intermittent strike-slip deformation. SINGH\_SAW model predicts the whole Afghan Block in the strike-356 slip regime (Figure 6g-h). S40RTS and S2.9\_S362 predict higher stress magnitude in NW parts of the 357 Zagros Orogeny system and Central Iran compared to other models. 358

The misfit between observed and predicted  $S_{Hmax}$  is found to be much lower for mantle convection 359 models (0.54-0.57) (Figure 7 left panel), than those of GPE only models (Figure 5 left panel), evidently 360 showing the importance of mantle flow. The lowest average misfit is observed for SAW642AN (0.54) 361 (Figure 7d). Though the misfit increases in the east, Lut block, and near MSZ. The correlation of 362 predicted deviatoric stresses with GSRM strain rates improves over GPE only models (Figure 7 middle 363 panel), with SAW642AN yielding the highest correlation coefficient (0.91) (Figure 7e). Correlation 364 drops below 0.4 parts of central Iran. S40RTS performs predicts the plate velocities closest to the 365 observed one, out of all models, with the least RMS error ( 6.20 mm/yr) between predicted and observed 366 plate velocities (Figure 7c). On the other hand, SAW642AN and 3D2018\_S40RTS models show high 367 misfits (rms error  $\sim 10 mm/yr$ ), as they are unable to match observed plate velocities in Zagros-Iran 368 plateau, both in orientations and magnitude (Figures 7f & i). 369

As discussed above, mantle convection models perform better in predicting deviatoric stresses in the study area which is evident by high correlation between predicted stresses and observed strain rates; and low misfits between observed and predicted  $S_{Hmax}$ . However, the error in predicting plate velocities is higher for mantle convection models than in GPE only models. GPE only models perform slightly better in predicting the orientation and magnitude of velocity vectors. Thus, As there are still significant misfits in fitting the observables, we added the deviatoric stresses predicted from GPE differences and Mantle <sup>376</sup> convection models to constrain the total stress field in the Zagros-Iranian plateau that may account for
 <sup>377</sup> both forces.

We also ran S40RTS model with LAB (Lithosphere-Asthenosphere boundary) at 150 and 200 km (Figure S2g-h). Similar to GPE models, the fit to observed data shows an improvement when LAB is at 200 km, though the stress patterns do not change significantly (Table S2).

#### **4.3** Stress and deformation by GPE and Mantle convection

Adding mantle contributions to GPE only models led to significant changes in total deviatoric stresses 382 for all models (Figure 8,9,10). There is a significant increase in total stress magnitude of the entire study 383 area; except for north of MRF and SE of central Iran, which show slightly lower stresses (< 16 MPa) 384 for combined models of CRUST2 and mantle convection (Figure 8). These models show predominant 385 compression in most of Zagros, SSZ, UDMA, NW and central Iran, except for the strike-slip type of 386 deformation in NW parts. The joint models of CRUST1 and mantle convection predict higher stresses 387 (> 25 MPa) in NW Iran and at MFF (Figure 9). Interestingly, the stresses drop below 20 MPa towards 388 the north of HZF, MRF till the south Capsian. The combined models of CRUST1 and mantle convection 389 show compressional stresses are dominant in the study area, with occasional strike-slip faulting in the 390 north-west (Figure 9 right panel). The stresses predicted by combined models of LITHO1 and mantle 391 convection models are higher in magnitude than other models in the study area (> 25 MPa) (Figure 10). 392 S40RTS+litho and S2.9\_S362+litho models show high stresses in Zagros (>50 MPa)(Figure 10a,g). 393

The combined models show a lower misfit between observed and predicted  $S_{Hmax}$  (Figure 11), especially when compared to GPE only models (Figure 5 left panel). SAW642AN+litho showed the lowest average misfit of 0.47 (Figure 11f). Interestingly, SAW642ANcr2 and 3D2018\_S40RTScr2 show low misfits in the Zagros-Iranian plateau region, despite not having the lowest average misfit (Figures 11d & g). The higher misfits in NW Iran and SE of the central Iran block observed for GPE only models get reduced significantly due to the addition of mantle derived stresses, referring to the importance of mantle convection in these areas.

As we look at the correlation between predicted stress tensors and GSRM strain rate tensors, the over-401 all correlation is better for combined models (Figure 12), especially for combined models of LITHO1 402 and mantle convection (Figure 12 right panel). A high average correlation coefficient of 0.94 is ob-403 served for SAW642AN+litho, 3D2018\_S40RTS+litho as well as S2.9\_S362+LITHO1 (Figures 12f, i & 404 1). Despite an overall improvement in correlation between observed strain tensors and predicted devia-405 toric stresses, the correlation is found to be much poor in areas such as NW parts of Zagros and east of 406 central Iranian block, for combined models of mantle convection and GPE only models of CRUST2 & 407 CRUST1 (Figure 12 left and middle panels). In NW Zagros, mantle only models are found to perform 408

much better, as they show better correlation (Figure 7 middle panel), thus suggesting mantle derived
stresses are needed to be much higher than those from GPE to explain the observed deformation in these
areas.

Again the combined models of GPE and mantle tractions give lower rms errors, when predicted 412 plate velocities are compared to the observed ones. S40RTScr2 shows the least rms error (3.28 mm/yr) 413 and the least average angular misfit  $(3.0^{\circ})$  between predicted and observed plate velocities (Figure 13a). 414 Relatively the combined models of S40RTS/S2.9\_S362 and GPE perform much better than other models 415 in predicting the orientation and magnitudes of plate velocities. Significant misfits are observed for 416 SAW642ANcr1 and 3D2018\_S40RTScr1 models. The joint models of S40RTS and GPE for thicker 417 lithosphere do not offer any significant changes in stresses and their fit to observed data (Table S2) 418 (Ghosh et al., 2009; Jay et al., 2018; Hirschberg et al., 2018). Thus, considering the lithosphere base at 419 100 km appears to be a satisfactory approach. 420

## 421 **5 Discussion**

The Zagros-Iranian plateau region is formed due to the convergence of Arabian plate towards the Eura-422 sian plate. Zagros mountain belt demarcates the southwestern boundary of the deformation zone, 423 whereas, it is bounded by the Makran subduction zone in the southeast and by Afghan Block in the 424 east. Kopet-Dagh and Arborz act as this region's northeastern and northern boundaries (Irandoust et al., 425 2022). We modeled the stresses and deformation parameters in the study area by solving the force bal-426 ance equation using the finite element method for a global grid of  $1^{\circ} \times 1^{\circ}$  resolutions, considering two 427 primary sources of stresses; GPE and mantle tractions. GPE was calculated using the thickness and den-428 sity variation from the different global models like CRUST1.0, CRUST2.0 and LITHO1.0. The shear 429 tractions were computed from density derived mantle convection model. 430

The magnitude of stresses due to GPE variations was below 15 MPa in the Iranian plateau for 431 CRUST2 and CRUST1 models (Figures 4a & c). However, LITHO1 model predicted higher stresses 432 (> 30 MPa) with predominant compression in parts of the Zagros-Iran region and Afghan block. Most of 433 the convergence of Arabian and Eurasian plates has been accommodated through shortening across Za-434 gros (Irandoust et al., 2022; Khodaverdian et al., 2015). Walpersdorf et al. (2006); Hessami et al. (2006) 435 suggested nearly pure N-S shortening of  $8 \pm 2mm/yr$  in southeastern Zagros. The convergence occurs 436 perpendicular to the simply folded mountains and is restricted to the shore of Persian Gulf. Earthquake 437 focal mechanisms also show reverse faulting within this area (Berberian, 1995; Hatzfeld et al., 2010; 438 Hatzfeld & Molnar, 2010; Irandoust et al., 2022). In our study, LITHO1 model predicted thrust mode 439 of faulting within Zagros, which is consistent with these results. In NW Zagros, Hatzfeld et al. (2010); 440

Hatzfeld & Molnar (2010); Jackson & McKenzie (1984); Khorrami et al. (2019); Talebian & Jackson 441 (2002) and various others have suggested partitioning of deformation. The oblique shortening is par-442 titioned into strike-slip faulting that is accommodated by MRF, while shortening occurs perpendicular 443 to the mountain belt (Hatzfeld et al., 2010; Hatzfeld & Molnar, 2010; Jackson & McKenzie, 1984; 444 Khorrami et al., 2019; Talebian & Jackson, 2002). On considering lithospheric models only, we pre-445 dicted the normal mode of faulting to be dominant in this area for CRUST2. On the other hand, CRUST1 446 model predicted strike-slip components in the northern segment of MRF, while LITHO1 showed thrust 447 type of deformation in this area. Interestingly, the misfits of predicted parameters with various observa-448 tions of  $S_{Hmax}$ , strain rates and plate velocities were found to be lowest for LITHO1 model, thus arguing 449 for thrust type of deformation in this area. SSZ in north of MZT consists of various thrust systems 450 (Alavi, 1994). CRUST1 predicted thrust mode of faulting in this region, while CRUST2 and LITHO1 451 models showed intermittent strike-slip type of faulting. Alborz as well as Kopeh Dagh in the north 452 has also been subjected to reverse faulting (Allen et al., 2003; Hatzfeld & Molnar, 2010; Hollingsworth 453 et al., 2010; Irandoust et al., 2022; Khodaverdian et al., 2015), which has also been shown by CRUST1 454 and LITHO1 models. Models predicting thrust in Talesh mountains show low misfits to observation 455 suggesting thrusting of the mountain range over the basin with slip vectors directed towards the South 456 Caspian Sea (Irandoust et al., 2022). The N-S convergence in Kopeh-Dagh range iswas predicted by 457 LITHO1 model considering the contribution from lithospheric density and topographic variations only. 458 The shearing between Central Iran and Afghan Block caused due to varying rates of shortening across 459 the Zagros, Alborz and Caucasus, is accommodated by strike-slip faults near Lut block boundaries 460 (Khorrami et al., 2019; Vernant et al., 2004; Walpersdorf et al., 2014). Again, LITHO1 model predicted 461 similar strike-slip deformation in these areas; however, CRUST2 and CRUST1 failed to do so. 462

The stresses predicted using basal tractions were mostly compressional in southeastern Zagros owing 463 to the convergence of Arabia-Eurasia (Figure 6). However, all models, except SAW642AN predicted 464 strike-slip type of deformation in the northwestern Zagros (MRF), which concurs with the results from 465 various studies (Hatzfeld et al., 2010; Hatzfeld & Molnar, 2010; Jackson & McKenzie, 1984; Khorrami 466 et al., 2019; Talebian & Jackson, 2002). The mantle derived stress parameters showed a better fit to 467 observables than those from GPE variations (Figures 7 left and middle panel), though the correlation 468 dropped below 0.5 in Central Iran. Here, mantle convection models foundpredicted compressional type 469 of deformation, while Baniadam et al. (2019); Khorrami et al. (2019) suggested that strike-slip faulting 470 along the fault system bounding Lut Block. The velocity misfits were very high for all models except 471 S40RTS (Figure 7 right panel). Although we used four tomography models to compute the mantle-472 derived stresses, the stress regimes for all models are found to be similar, with varying magnitudes. Such 473 results suggest that nearly all four seismic tomography models are relatively consistent in predicting the 474

475 stresses in this region.

Adding the GPE derived stresses to those from the mantle to obtain the total lithospheric stress field 476 showed a notable improvement in constraining the observed deformation parameters. The final stress 477 regimes also varied significantly depending on particular combinations of GPE and mantle convection 478 models. All joint models of CRUST2 and mantle tractions showed lower magnitudes of stresses (< 15 479 MPa) in the north of MRF, Tehran and southern Lut block. The stresses showed an obvious increase 480 in these areas for other models. Significantly higher stresses (> 30 MPa) were also observed near the 481 collisional front (MFF) for all models. On comparing with observations, combined models of CRUST2 482 and mantle tractions showed significant improvement in fit, except in areas north of MRF and Tehran. 483 CRUST1 model when added with mantle contribution, predicted thrust faulting along the faults bound-484 ing Lut Block, leading to poor correlation (< 0.5). On the other hand, combined LITHO1 and mantle 485 convection models gave a much better fit in this area, as they predicted strike-slip faulting. The use of 486 different mantle convection models is much less sensitive in the Iran-Zagros region, as most models can 487 match various surface observables reasonably well. 488

On running various models and comparing the stresses in Zagros-Iran, we try to explain the relative roles of GPE and mantle tractions in causing observed deformation. The contributions from both sources vary significantly among different models. However, these variations arise mainly from GPE only models, which may be due to uncertainties in crustal models of this area. Another interesting observation from this study is that the role of GPE in the study region may not be that significant, as mantle derived stresses were able to explain many of the deformation indicators. To get a quantitative constraint on the best model, we computed a total error as given below:

$$Total \, error = S_{Hmax} \, error + 1 - C_{strain} + V_{rms} \tag{7}$$

 $S_{Hmax}$  error in the above equation is calculated as mentioned in section 3.4, while  $C_{strain}$  is the correlation computed using equation 6.  $V_{rms}$  is the rms error between predicted and observed velocities. The total errors calculated using equation 7 have been tabulated in Table 1. S40RTScr2 is found to have the lowest error.

<sup>500</sup> We also calculated plate velocities with respect to the Eurasian plate (Figure 14) and compared them <sup>501</sup> with observed GPS velocities relative to Eurasia. The GPS velocities were obtained from various studies <sup>502</sup> conducted in the study this area (ArRajehi et al., 2010; Bayer et al., 2006; Frohling & Szeliga, 2016; <sup>503</sup> Khorrami et al., 2019; Masson et al., 2006, 2007; Raeesi et al., 2017; Reilinger & McClusky, 2011; <sup>504</sup> Vernant et al., 2004). GPS measurements show a northward convergence rate of  $\sim 22mm/yr$  for Arabia <sup>505</sup> relative to Eurasia (Reilinger et al., 2006; Vernant et al., 2004), however, it varies significantly along <sup>506</sup> the Zagros. The southeastern Zagros show the highest convergence rates of  $\sim 25$  mm/yr oriented in

Model	S <sub>Hmax</sub> misfit	Strain rate correlation	RMS error (mm/yr)	Angular misfit	Total error
CRUST2	0.77	0.69	7.32	5.5	3.07
CRUST1	0.64	0.87	7.44	8	2.78
LITHO1	0.59	0.92	8.51	9	2.81
S40RTS	0.57	0.88	6.2	4.6	2.51
SAW642AN	0.54	0.91	11.35	13	3.06
3D2018_S40RTS	0.56	0.88	9.44	9.7	2.92
S2.9_S362	0.57	0.88	8.29	9	2.81
S40RTScr2	0.48	0.92	3.28	3	1.75
SAW642ANcr2	0.49	0.92	4.77	5.5	2.13
3D2018_S40RTScr2	0.49	0.91	4.06	4.5	1.98
S2.9_S362cr2	0.48	0.92	4.24	5.1	2.00
S40RTScr1	0.51	0.92	4.29	5.5	2.05
SAW642ANcr1	0.5	0.92	7.39	9.6	2.58
3D2018_S40RTScr1	0.51	0.91	6.35	8.2	2.45
S2.9_S362cr1	0.51	0.92	4.78	6.6	2.15
S40RTS+litho1	0.49	0.93	4.52	6.1	2.07
SAW642AN+litho1	0.47	0.94	6.42	7.4	2.39
3D2018_S40RTS+litho1	0.48	0.94	5.62	7.2	2.27
S2.9_S362+litho1	0.48	0.94	5.8	8.3	2.30

Table 1: Summary of quantitative comparison of predicted results of various models with observed data.

north-northeast directions. GPS vectors are oriented northward in Central Zagros, which transitions 507 north-northwest in NW parts of Zagros with the lowest convergence rates of  $\sim 18$  mm/yr (Hatzfeld & 508 Molnar, 2010; Hatzfeld et al., 2010; Khorrami et al., 2019). Vernant et al. (2004) suggested that MSZ 509 accommodates most of the shortening  $(19.5 \pm 2 \text{ mm/yr})$  in the east of  $58^{\circ}E$ , while fold and thrust belts of 510 Zagros, Alborz and Caucasus collectively accommodate the shortening in west of 58°E. GPS velocities 511 in the east of Iran (Afghan Block) are very small in magnitude. To the west, velocities increase showing 512 westward rotation of Antolia (Khorrami et al., 2019; Reilinger et al., 2006). The northern part of Iran 513 shows that GPS vectors are aligned towards the northeast. We found that the combined model of S40RTS 514 and CRUST2 can approximately match the GPS velocities (Figure 14a). Predicted plate velocities with 515 respect to the fixed Eurasian plate show a northward movement of 2-3 cm/yr in southeastern Zagros. 516 The plate moves in NNE direction east of central Zagros ( $53^{\circ}$  E). On the other hand, west of  $53^{\circ}$  E 517 shows a movement in NNW direction, becoming much more prominent in the north. However, the 518 convergence rates in the east of Iran i.e. Lut Block as well as Afghan Block, is predicted to be much 519 higher ( $\sim 1 - 2cm/yr$ ) than those suggested by various observations. Plate velocities predicted by joint 520 models, S40RTScr1 and S40RTS+LITHO1 show nearly N-S contraction of of very high magnitudes 521 (4-5 cm/yr) throughout the region (Figure S3), which suggests much higher rates of deformation than 522 those suggested by above-mentioned studies. 523

<sup>524</sup> We also used shear wave splitting measurements to further study the deformation in the Zagros-Iran

region by comparing them with  $S_{Hmax}$  (Figure 14b). The fast polarization directions (FPDs) are the in-525 dicators of seismic anisotropy. We consider two primary causes of seismic anisotropy; induced by stress 526 and due to structure of the region (Yang et al., 2018). If the FPDs are parallel to  $S_{Hmax}$  orientations, it 527 suggests that anisotropy is associated with stress. On the other hand, latter kind of anisotropy is related 528 with the alignment of fault, fast axes of minerals that may cause polarization, and sedimentary bedding 529 planes. The FPDs in our study were obtained from Sadeghi-Bagherabadi et al. (2018); Kaviani et al. 530 (2009, 2021). The FPDs are subparallel to  $S_{Hmax}$  orientations in NW Zagros, Arabian plate, northern 531 Iran and MSZ. Such a correlation between both indicates that anisotropy in this region may be stress 532 induced. Additionally, the correlation of  $S_{Hmax}$  orientations and FPDs argues for a good coupling be-533 tween lithosphere and mantle in those areas. In contrast, Sadeghi-Bagherabadi et al. (2018) showed 534 FPDs parallel to the strike of the fault (sub-parallel to  $S_{Hmax}$  directions of CRUST2), In NW Zagros, 535 Sadeghi-Bagherabadi et al. (2018) also showed FPDs parallel to the strike of the fault, suggesting seis-536 mic anisotropy mainly reflects the deformation in the lithospheric mantle. Again, FPDs are subparallel 537 to the strike of range in northeastern Iran, eastern Kopeh Dagh and central Alborz indicating structure-538 induced anisotropy caused by strong shearing along the strike-slip faults (Gao et al., 2022; Kaviani et al., 539 2021). 540

To explore the relative roles of lithospheric and mantle derived stresses, we compared the deviatoric 541 stresses from CRUST2 to those from S40RTS. We performed a correlation between both stresses by 542 using equation 5 and found a high correlation (> 0.5) near MSZ and central Zagros (Figure 14c). The 543 correlation degrades north of the simply folded mountains and NW Iran. The stresses are anti-correlated 544 in northwestern parts of higher Zagros, north of MRF and Tehran, as CRUST2 predicted NNE-SSW 545 tension (Figure 4b) as opposed to the strike-slip faulting predicted by S40RTS (Figure 6b). Lut Block 546 also shows a slight anticorrelation between stresses ( $\sim -0.5$ ), as the stresses predicted by CRUST2 547 are very low. The log of the ratio of second invariants of deviatoric stresses from GPE variations  $(T_1)$ 548 to that of mantle tractions  $(T_2)$  is plotted in Figure 14d. Positive values of logarithmic ratio suggests 549 the dominance of GPE derived stresses over mantle ones, as observed in the south of the collisional 550 boundary (MFF). The ratio is negative in most parts of the Iranian plateau and Zagros, indicating that 551 the magnitude of mantle derived stresses is are higher than that of those from GPE, especially in higher 552 Zagros and central Iran (Figure 14d). 553

The deformation in the Zagros-Iran plateau region has been found to exhibit various similarities to another similar complex collision zone, i.e. the Himalaya-Tibetan plateau region as both continental collisions went through many of the same processes. The high topography in both collisions reflects ongoing crustal deformation through crustal thickening and shortening. However, there are differences in convergence rates, total amounts of convergence and various stages of development of the Zagros-Iran

and Himalaya-Tibet regions (Hatzfeld & Molnar, 2010). Singh & Ghosh (2020) studied the deformation 559 in the Himalaya-Tibet region by joint modeling of lithosphere and mantle. They showed that GPE 560 plays a crucial role in the ongoing deformation of the India-Eurasia collision zone, as it is leads to the 561 observed E-W extension in Tibetan plateau. In contrast, we found that GPE has a much lesser role in the 562 Zagros-Iran plateau region (Figure 14d), and no normal mode of faulting is observed in this area. In the 563 Zagros-Iran plateau region, mantle convection appears to be the primary driver of deformation in most 564 parts as discussed above. Despite these differences, numerical models argue for a good coupling between 565 the lithosphere and mantle in both collision zones, which is also supported by seismic anisotropy studies 566 in both regions (Kaviani et al., 2021; Singh et al., 2016; Sol et al., 2007). 567

## **6 Conclusion**

The Zagros-Iranian plateau region has large deformations along and across the collision zones. There-569 fore, we conducted numerical simulation studies for stress and deformations. The stresses predicted 570 in this region were primarily compressional, with magnitudes lower than 30 MPa. The southeastern 571 boundary of Zagros was found to be under high stress which is also reflected by higher convergence 572 rates. Mantle convection models wereare able to constrain most observations in the Iranian plateau. 573 However, the misfits with observations wereare much larger in the east of Iran, when only mantle con-574 tributions wereare considered. The combined models of lithosphereie and mantle-derived stresses can 575 explaingive a better fit to surface observables in most of the area, suggesting a good lithosphere-mantle 576 coupling, except for east of Iran. The fit between both predicted and observed data increases after 577 considering mantle derived stresses. The shearing in those areas wasis predicted by lithospheric models, 578 though variation in lithospheric and density structure given by these models lead to varying degree of 579 misfits. Hence, there is a need for better constraint on lithospheric structure in this area. 580

The mantle derived stresses were found to be much higher than lithospheric stresses, thus the over-581 all stress regimes predicted by combined models were more biased towards the compressional type of 582 stresses. This caused our combined models to predict thrust mode of faulting in most cases, especially 583 when lithospheric derived stresses were computed from CRUST1 and LITHO1 models. CRUST2 model 584 predicted more extensional stress in the Iranian plateau, which in turn balanced the effect of compres-585 sional stresses predicted by mantle convection models; hence leading to prominence of strike-slip mode 586 of faulting in the northwestern parts of study region. The rate of convergence of Arabia relative to a 587 fixed Eurasia was found to vary along the Zagros orogeny in a similar way to GPS measurements. 588

## **Open Research Section**

We used three models, namely CRUST1.0, CRUST2.0, and LITHO1.0, for obtaining the data of crustal 590 and lithospheric structure, which are required as inputs in finite element models. We downloaded these 591 three models and the seismic tomography models used in mantle convection codes from the Incorporated 592 Research Institutions for Seismology (IRIS) Earth Model Collaboration repository (http://ds.iris. 593 edu/ds/products/emc-earthmodels/). The strain rate model, GSRMv2.1 was obtained from http: 594 //geodesy.unr.edu/GSRM/. World Stress Map Website (https://www.world-stress-map.org/) 595 provides the  $S_{Hmax}$  orientations and type of faulting, which were used to perform a quantitative com-596 parison with predicted results. GPS velocities relative to Eurasia were taken from ArRajehi et al. 597 (2010); Bayer et al. (2006); Frohling & Szeliga (2016); Khorrami et al. (2019); Masson et al. (2006, 598 2007); Raeesi et al. (2017); Reilinger & McClusky (2011); Vernant et al. (2004). We also used seismic 599 anisotropy data from Sadeghi-Bagherabadi et al. (2018); Kaviani et al. (2009, 2021). 600

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**Figure 1:** Tectonic overview of Central Eurasia. Abbreviations: CF: Chaman Fault; MSZ: Makran Subduction Zone; MZT: Main Zagros Thrust; HZF: High Zagros Fault; MFF: Mountain Front Fault; SSZ: Sanandaj Sirjan Zone; UDMA: Urumieh-Dokhtar Arc; MRF: Main Recent Fault.



**Figure 2:** Thickness and density variations of different layers in all three crustal and lithospheric models: CRUST2(Left panel), CRUST1(Middle Panel) and LITHO1(Right panel)



**Figure 3:** (a) Most compressive horizontal principal axes ( $S_{Hmax}$ ) from WSM (Heidbach et al., 2016). Red indicates normal fault regime, blue indicates thrust regime, whereas green denotes strike-slip regime, (b) Observed plate velocities in a no-net-rotation frame of reference from Kreemer et al. (2014) plotted on top of second invariant of strain rate tensors obtained from Kreemer et al. (2014) plotted on  $1^{\circ} \times 1^{\circ}$  grid.



**Figure 4:** (Left Panel) Deviatoric stresses predicted from GPE variations, plotted on top of their second invariants. The compressional stresses are denoted by solid black arrows, while white arrows show tensional stresses.  $S_{Hmax}$  axes predicted from GPE variations are plotted in right panel. Red denotes tensional regime, blue is for thrust and green for strike-slip regime.



**Figure 5:** (Left Panel) Total misfit between observed and predicted  $S_{Hmax}$  from GPE variations. Correlation coefficients between strain rate tensors obtained from Kreemer et al. (2014) and deviatoric stresses predicted using GPE variations are shown in middle panel, with average regional correlation coefficients given on bottom right of each figure. (Right panel) Observed velocities (black) and predicted plate velocities(white) from GPE variations in NNR frame, plotted on the top of angular misfit between both.



**Figure 6:** (Left Panel) Deviatoric stresses predicted using mantle tractions derived from various tomography models for GHW13 viscosity structure, plotted on second invariant of deviatoric stresses. The white arrows denote tensional stresses, and black arrows indicate compressional stresses.  $S_{Hmax}$  predicted from mantle tractions are shown in right panel. Red denotes tensional regime, blue is for thrust and green is for strike-slip regime.



**Figure 7:** Parameters predicted from mantle tractions and their comparisons with observables. (Left panel) Total misfit between  $S_{Hmax}$  obtained from WSM (Heidbach et al., 2016) and those predicted using mantle tractions derived from various tomography models using GHW13 viscosity structure. Correlation coefficients between strain rate tensors obtained from Kreemer et al. (2014) and deviatoric stresses predicted using basal tractions are shown in middle panel, with average regional correlation coefficients given on bottom right of each figure. (Right pannel) Observed velocities (black) and plate velocities predicted using mantle tractions (white) in NNR frame plotted on the top of angular deviation between both.



**Figure 8:** (Left panel) Deviatoric stresses predicted using combined effects of GPE computed from CRUST2 and mantle tractions derived from various tomography models plotted on top of their second invariants. The white arrows denote tensional stresses, and black arrows indicate compressional stresses. The right panel shows  $S_{Hmax}$  predicted from these models. The red lines denote tensional regime, blue is for thrust and green is for strike-slip regime.



**Figure 9:** (Left panel) Deviatoric stresses (a-d) predicted using combined effects of GPE computed from CRUST1 and mantle tractions derived from various tomography models plotted on top of their second invariants. The white arrows denote tensional stresses, and black arrows indicate compressional stresses. The right panel shows  $S_{Hmax}$  predicted from these models. The red lines denote tensional regime, blue is for thrust and green is for strike-slip regime.



Figure 10: (Left panel) Deviatoric stresses (a-d) predicted using combined effects of GPE computed from LITHO and mantle tractions derived from various tomography models plotted on top of their second invariants. The white arrows denote tensional stresses, and black arrows indicate compressional stresses. The right panel shows  $S_{Hmax}$  predicted from these models. The red lines denote tensional regime, blue is for thrust and green is for strike-slip regime.



**Figure 11:** Total misfit between observed  $S_{Hmax}$  from WSM (Heidbach et al., 2016) and  $S_{Hmax}$  predicted using combined effects of GPE computed from different crustal models and mantle tractions derived from various to-mography models.



**Figure 12:** Correlation coefficients between strain rate tensors from Kreemer et al. (2014) and deviatoric stress tensors predicted using combined effects of GPE computed from different crustal models and mantle tractions derived from various tomography models. Average correlation coefficient is given in right lower corner of the figure.



**Figure 13:** Plate velocities predicted using combined effects of GPE computed from different crustal models and mantle tractions derived from various tomography models plotted on top of angular misfit ( $\theta$ ). Black arrows represent observed NNR velocities (Kreemer et al., 2014) and white ones denote predicted velocities.



**Figure 14:** Predicted parameters of best fit model, S40RTScr2. (a) GPS (blue) and predicted (red) plate velocities with respect to a fixed Eurasian plate, (b) FPDs (blue) and  $S_{Hmax}$  (red) are plotted for the best fit model, (c) Correlation between deviatoric stresses predicted from GPE and mantle convection models, and (d) ratio  $(T_1/T_2)$  of second invariant of deviatoric stresses from GPE  $(T_1)$  to those from mantle tractions  $(T_2)$ .



**Figure S1:** (Left) Plot of lithospheric viscosity in the study region that is used in finite element models. Right panel shows GHW13(red) and SH08 (blue) viscosity structures used in mantle convection models.



**Figure S2:** (a-f)Deviatoric stresses predicted using GPE models for lithosphere base at 150 km (left) and 200 km (right). (g-h) Mantle derived stresses from S40RTS tomography model for GHW13 viscosity structures, when LAB is at 150 km (left) and 200 km (right). The background plot shows the second invariant of deviatoric stresses. The white arrows denote tensional stresses, and black arrows indicate compressional stresses.



**Figure S3:** (Left Panel) GPS (blue) and predicted (red) plate velocities with respect to a fixed Eurasian plate. Right Panel shows plot of FPDs in blue and  $S_{Hmax}$  in red.

Model	SHmax misfit	Strain rate correlation	RMS error (mm/yr)	Angular misfit	Total error
S40RTS+SH08	0.58	0.9	5.68	6	2.42
SAW642AN+SH08	0.58	0.88	17.41	22	3.56
3D2018_S40RTS+SH08	0.58	0.88	8.68	9.2	2.86
\$2.9_\$363+\$H08	0.54	0.89	10.38	14	2.99
S40RTS+SH08cr2	0.52	0.91	3.81	3.3	1.95
SAW642AN+SH08cr2	0.56	0.89	5.38	5.1	2.35
3D2018_S40RTS+SH08cr2	0.54	0.89	4.15	3.3	2.07
\$2.9_\$362+\$H08cr2	0.52	0.92	5.14	5.8	2.24
S40RTS+SH08cr1	0.54	0.92	4.8	6.1	2.19
SAW642AN+SH08cr1	0.54	0.91	8.61	10.7	2.78
3D2018_S40RTS+SH08cr1	0.56	0.91	6.3	7.9	2.49
S2.9_S362+SH08cr1	0.55	0.91	5.82	7.6	2.40
S40RTS+SH08+litho	0.52	0.94	5.79	7.4	2.34
SAW642AN+SH08+litho	0.51	0.94	8.05	8.7	2.66
3D2018_S40RTS+SH08+litho	0.53	0.94	6.61	8.2	2.48
S2.9_S362+SH08+litho	0.53	0.94	7.61	10.1	2.62

**Table S1:** Summary of quantitative comparison of predicted results of various models with observed data for SH08 viscosity model (Steinberger & Holme, 2008).

Table S2: Qua	ntitative comparison	n of fit to the ol	bserved data for	varying LAB depths.
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Model/LAB Depth	S <sub>Hmax</sub> error		Strain Rates Correlation			Velocity rms error			
	100 km	150 km	200 km	100 km	150 km	200 km	100 km	150 km	200 km
CRUST2	0.77	0.64	0.6	0.69	0.83	0.87	7.32	5.85	5.69
CRUST1	0.64	0.61	0.6	0.87	0.9	0.9	7.44	8.59	9.28
LITHO1	0.59	0.56	0.56	0.92	0.93	0.93	8.51	9.03	9.45
S40RTS	0.57	0.56	0.54	0.88	0.89	0.9	6.2	5.9	6.06
S40RTScr2	0.48	0.48	0.49	0.92	0.92	0.93	3.28	5.24	3.82
S40RTScr1	0.51	0.52	0.53	0.92	0.92	0.92	4.29	9.6	9.28
S40RTS+litho1	0.49	0.5	0.51	0.93	0.93	0.94	4.52	9.03	9.45