An assessment of long duration geodynamo simulations using new paleomagnetic modeling criteria (QPM)

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Abstract:

Long-term temporal variations of the magnetic field (timescales > 10 Myr), characterized from paleomagnetic data, have been hypothesized to reflect the evolution of Earth’s deep interior and couplings between the core and mantle. By tying observed changes in the paleomagnetic record to mechanisms predicted from numerical geodynamo simulations, we have a unique tool for assessing changes in the deep interior back in time. However, numerical simulations are not run in an Earth-like parameter regime and assessing how well they reproduce the geomagnetic field is difficult. Criteria have been proposed to determine the level of spatial and temporal agreement between simulations and observations spanning historical and Holocene timescales, but no such criteria exist for longer timescales.

Here we present a new set of five criteria (Quality of Paleomagnetic Modeling criteria, QPM) that assess the degree of semblance between a simulated dynamo and the temporal and
spatial variations of the long-term (~ 10 Myr) paleomagnetic field. These criteria measure inclination anomaly, virtual geomagnetic pole dispersion at the equator, latitudinal variation in virtual geomagnetic pole dispersion, normalized width of virtual dipole moment distribution, and dipole field reversals. We have assessed 46 geodynamo simulations using the QPM criteria. The simulations have each been run for the equivalent of at least ~300 kyr, span reversing and non-reversing regimes, and include either homogeneous or heterogeneous heat flux boundary conditions. We find that none of our simulations reproduce all salient aspects of the long-term paleomagnetic field behavior for the past 10 Myr. Nevertheless, our simulations bracket Earth values, suggesting that an Earth-like simulation is feasible within the available computationally accessible parameter space. This new set of criteria can inform future simulations that aim to reproduce all aspects of Earth’s long-term magnetic field behavior.

**Keywords:** Numerical geodynamo simulations, paleosecular variation, time average magnetic field, paleomagnetism

1. Introduction

The geomagnetic field has been a fundamental feature of the Earth for the past 3.5 billion years (Biggin et al., 2011, 2015; Tarduno et al., 2010) and may have been active since the Hadean (Tarduno et al., 2015). Originating in Earth’s core and extending into space, the magnetic field shields the atmosphere from erosion by the solar wind, allowing for the preservation of liquid water on the surface and ultimately habitability (Tarduno et al., 2014). Thus, the geomagnetic field is a link between surface, interior, and exterior processes back through geologic time. The magnetic field observed at Earth’s surface contains contributions primarily from internal sources. Temporal variations (secular variation) and spatial variations in
the internally generated field can be characterized through direct observations using surface,  
satellite, and aeromagnetic measurements for the last few hundred years (historical record) and  
indirectly via paleomagnetic/archeomagnetic measurements going further back in time. These  
variations provide insight into the magnetohydrodynamic processes that occur in the outer core,  
and into how these processes may be affected by boundary conditions imparted at the mantle and  
inner core interfaces (Aubert et al., 2010; Olson et al., 2013). The similarity between the  
timescales observed for long-term variations in the magnetic field, e.g. the timescale for reversal  
frequency variability, to those of convective overturn in the mantle (200 Myr), has led to the  
hypothesis that long-term magnetic field variations are a result of external forcing mechanisms  
and reflect the evolution of Earth’s deep interior (Biggin et al., 2012; Jones, 1977; McFadden  
and Merrill, 1984). If observed variations in the long-term magnetic field can be tied to  
mechanisms predicted from numerical geodynamo simulations, it would then be possible to  
evaluate changes in the deep interior going back in geologic time, adding a crucial dimension to  
our understanding of Earth’s evolution.  

In the last three decades, significant advances have been made in the field of numerical  
geodynamo modeling. These simulations have succeeded in capturing the main features of the  
Earth’s magnetic field, such as a dipole dominated field and polarity reversals (e.g. Christensen  
and Wicht, 2015; Glatzmaier and Coe, 2015; Glatzmaier and Roberts, 1995), in addition to  
aspects of historical secular variation (Bloxham, 2000; McMillan et al., 2001) such as westward  
drift (Christensen and Olson, 2003) and weak activity in the Pacific hemisphere (e.g. Aubert et  
al., 2013; Davies et al., 2008; Gubbins et al., 2007; Mound et al., 2015). Furthermore,  
simulations have been used to make predictions about magnetic field behavior including  
estimates of internal field strength and core flow speed (Christensen et al., 2009; Christensen and
Aubert, 2006), relations between field strength and reversal frequency (Olson, 2007), the role of core-mantle boundary heat flow in affecting field behavior and flow dynamics (Amit et al., 2015; Amit and Olson, 2015; Olson and Christensen, 2002; Olson et al., 2010) and time-average field morphology (Amit et al., 2015; Amit and Choblet, 2009; Davies et al., 2008; Gubbins et al., 2007). However, due to computational limitations, numerical dynamo simulations cannot yet run with the small diffusion coefficients that characterize the core fluid. In terms of non-dimensional numbers, the Ekman number $E$ (the ratio of viscous to Coriolis forces) and the magnetic Prandtl number $P_m$ (the ratio of viscous to magnetic diffusion) are many orders of magnitude larger than those estimated for Earth. Lowering $E$ to geophysical values of $10^{-15}$ is the main challenge.

Recent simulations that utilized millions of CPU hours have reached $E = 10^{-7}$ (Schaeffer et al., 2017) or $10^{-8}$ by parameterizing the smallest scales of the turbulence (Aubert et al., 2017), but were only run for short time periods and do not reverse. A key issue is then to determine to what degree a given simulation can be said to exhibit ‘Earth-like’ properties.

To assess whether a numerical dynamo simulation produces an Earth-like magnetic field, past studies have utilized observed behavior of the recent geomagnetic field derived from global time-dependent field models spanning historical and Holocene timescales, to develop criteria that can be used to assess the similarity between numerical simulations and Earth (Amit et al., 2015; Christensen et al., 2010; Davies and Constable, 2014; Mound et al., 2015). These global field models are constructed from satellite, observatory and survey magnetic field observations over the historical period 1590-1990 AD (gufm1; Jackson et al., 2000) and from archeomagnetic and paleomagnetic data, collected from archeological artifacts, sediments, and volcanic rocks for the past 10 to 100 kyr (e.g. Korte and Constable, 2011; Panovska et al., 2018). Existing criteria utilize large-scale properties of the field morphology (Christensen et al., 2010; Mound et al.,
2015; Amit et al., 2015) or the frequency content of the dipole moment time-series (Davies and Constable, 2014) derived from these global field models as the basis for assessing whether a numerical simulation reproduces Earth’s magnetic field behavior. In practice, these criteria have been used to assess the compliance of both short (< $10^5$ yr) and long duration (~$10^5$-$10^7$ yr) dynamo simulations with Earth-like behavior (e.g. Driscoll and Wilson, 2018), despite being based on features of the recent geomagnetic field. While it has been suggested that modern secular variation, as captured by global field models, is representative of expected variations over the entire history of the geodynamo, this is fundamentally uncertain (Johnson and McFadden, 2015). Furthermore, current criteria based on time-dependent field models do not include aspects of Earth’s long-term magnetic field behavior not observed in the Holocene, such as polarity reversals. To properly assess whether simulations behave like Earth on longer time scales (> $10^5$-$10^7$ yrs), we need to define a new set of criteria which can be used to assess how well numerical simulations reproduce paleomagnetic field behavior.

Here we present a new set of criteria to compare long-term behavior of numerical dynamo simulations with paleomagnetic observations: the Quality of Paleomagnetic Modeling (QPM) criteria. Criteria are assessed using a two-fold approach: 1) the calculation of a non-parametric misfit score ($\Delta Q_{PM}^i$) between simulated and Earth data, inspired by the approach used in Christensen et al. (2010), and 2) the assignment of a binary score ($Q_{PM}^f$), inspired by the paleomagnetic Q (Van der Voo, 1990) and QPI (Biggin and Paterson, 2014) approaches commonly used in the assessment of paleodirectional and paleointensity studies, respectively. Total misfit values, $\Delta Q_{PM}$, and total $Q_{PM}$ scores are evaluated over all criteria, where for each criterion that is met the total $Q_{PM}$ score increases by 1, to a maximum score of five. The utility of a two-fold method is as follows. First, this approach helps bring all simulations, regardless of the
parameter space in which they were run, to the same baseline, easing comparison between them. Second, the $\Delta Q_{PM}$ helps to quantify overall how close a simulation is to reproducing Earth’s paleomagnetic behavior, while the $Q_{PM}$ score highlights which specific aspects of the paleomagnetic field a simulation is reproducing well. Finally, the $Q_{PM}$ approach does not prescribe a strict threshold below which a simulation is deemed incompatible with paleomagnetic observations, which allows users to assess which of the paleo-field properties are most important to reproduce for their study. This permits users to get the most out of their simulations, which for timescales on the order of 1 Myr may have taken tens of thousands of CPU hours to run.

The chosen five criteria represent a range of commonly reported paleomagnetic observables that reflect temporal and spatial variations in the long-term magnetic field. Global time-dependent field models are not available for the timescales of interest here and our new criteria reflect the available data in the paleomagnetic record. For the purpose of this study, their Earth-like values are derived for the past 10 Myr as reported in the recent compilation of paleomagnetic directional data, PSV10 (Cromwell et al., 2018), and the paleointensity (PINT) database (Biggin et al., 2009, 2015) (Table 1). These criteria are assessed at Earth’s surface, requiring conversion of Gauss coefficients from geodynamo simulations into pseudo-paleomagnetic data. The five criteria address different aspects of the time-average and time-varying field and are as follows: inclination anomaly, virtual geomagnetic pole (VGP) dispersion at the equator, latitudinal variation of VGP dispersion, normalized width of virtual dipole moment (VDM) distribution, and dipole field reversals. We have assessed the compliance of our criteria with a large number of published (Davies et al., 2008; Davies and Constable, 2014; Davies and Gubbins, 2011; Gubbins et al., 2007), and new long-duration geodynamo simulations. These simulations span a wide parameter space that was chosen to best capture a
broad range of simulation behavior and serves to demonstrate the $Q_{PM}$ approach. Because we cannot predict *a priori* which simulations will reproduce Earth’s paleomagnetic field, we have chosen to explore this parameter space systematically.

In the following sections we will first review the observable properties of the paleomagnetic field that will be used as the foundation of the $Q_{PM}$ criteria and introduce the five $Q_{PM}$ criteria. We then outline how compliance with these criteria is met. Next, we use these criteria to assess how well our suite of 46 long-duration geodynamo simulations reproduce the Earth’s paleomagnetic field. We close with a discussion of the implications of our results, and how we foresee the utilization of these criteria in the future.

2. Paleomagnetic Modeling Criteria for Geodynamo Simulations ($Q_{PM}$)

In order to be effective, the criteria for assessing a numerical simulation should be objective and quantifiable (Christensen et al., 2010), and address a well-established property of the paleomagnetic field. We base our criteria solely on paleomagnetic observables and not on global time-dependent models (e.g. Panovska et al., 2018), which do not cover the time-frame of interest (>100 kyr), or statistical field models (e.g. Tauxe and Kent, 2004), which fail to reproduce paleomagnetic observations of paleosecular variation (PSV) and time-average field (TAF) behavior, or TAF models (e.g. Cromwell et al., 2018), which do not represent PSV.

Observations made directly from paleomagnetic datasets provide the most reliable representation of long-term magnetic field behavior and we therefore use them as the foundation of our criteria. Another constraint on viable criteria arises from limitations inherent in current dynamo simulations. Simulations spanning paleomagnetic timescales must run for long periods, which increases the computational cost and further limits the parameter range that can be accessed. We
therefore focus on large-scale features of the field as has been done in previous studies
(Christensen et al., 2010; Davies and Constable, 2014; Mound et al., 2015; Wicht and Meduri, 2016).

2.1 Paleomagnetic Basis for $Q_{PM}$ Criteria

To assess the behavior of the magnetic field on long time scales we are interested in both the geometry of the TAF in addition to temporal variations about the long term average (PSV). An overview of standard paleomagnetic observables is presented in the Supplementary Materials. Full vector records of the paleomagnetic field are sparse and unevenly reported. Therefore, in defining the $Q_{PM}$ criteria, magnetic directions and intensity are treated separately. The five criteria chosen for $Q_{PM}$ analysis discussed below are as follows: inclination anomaly (IncAnom), VGP dispersion (VGPa and VG Pb), normalized width of VDM distribution (VDMVar), and reversals (Rev).

2.1.1 Criterion Based on Time-Average Field Behavior

A fundamental assumption in paleomagnetic studies is that over a sufficiently long time period the field can be best approximated by a geocentric axial dipole (GAD), where inclination ($I_{GAD}$) is predicted to vary with latitude ($\lambda$) via the axial dipole equation

$$\tan I_{GAD} = 2 \tan \lambda.$$ (1)

However, paleomagnetic records show small, yet persistent, deviations from GAD (Cox, 1975; Cromwell et al., 2018; Johnson et al., 2008). The two parameters used to represent this offset in paleomagnetic studies are inclination anomaly and declination anomaly, defined as

$$\Delta I = \bar{I} - I_{GAD},$$ (2)

$$\Delta D = \bar{D}.$$ (3)
Here, $\bar{I}$ and $\bar{D}$ are the calculated Fisher mean (Fisher, 1953) inclination and declination values from measured samples. Note, the declination predicted from a GAD field is zero. Due to large gaps in spatial coverage in long-term paleomagnetic records, investigations are restricted to latitudinal structure only. In observational datasets, an accurate measure of $\Delta D$ is much harder to capture from paleomagnetic data than $\Delta I$, due to error in or absence of sample orientation, unrecognized tectonic rotation, and the expected long-term behavior of the longitudinal variation of the non-GAD field as captured by declination. Therefore, for our criteria we utilize $\Delta I$ ($\text{IncAnom}$), as one of our measures of TAF behavior.

The IncAnom criterion utilizes the maximum absolute median $\Delta I$ (calculated from 10° latitude bins) and its 95% confidence intervals as a measure of TAF behavior. We do not require that simulations match the observed latitudinal geometry of $\Delta I$, which we believe is justified since the latitudinal variation of $\Delta I$ is not well-constrained in the long-term magnetic field (Cromwell et al., 2018).

A measure of the mean field intensity or mean VDM (see equation 8 below) is most often used as a metric of TAF intensity. Dynamo simulations solve dimensionless equations and so scaling the results into a dimensional field strength is non-unique. Davies and Constable (2018) found that estimates of the local field intensity varied by a factor of 2-3 between two different magnetic field scalings within a given geodynamo simulation. Additionally, the ratio between the Elsasser and Lehnert number scalings commonly used in the literature is $\left(\frac{E}{Pm}\right)^{1/2}$ (Olson and Christensen, 2006), which at $E = 10^{-4}$ and $Pm = 1$ could produce a factor of 100 or more difference in the field strength. Due to these complexities, we do not include a direct measure of TAF behavior in regard to intensity in our $Q_{\text{PM}}$ criteria.

2.1.2 Criteria Based on Paleosecular Variation Behavior
VGP angular dispersion ($S$) is a commonly used metric to quantify paleosecular variation in the long-term paleomagnetic field. Using VGP dispersion allows for the estimation of paleosecular variation when detailed age control and time series data are unavailable. To mitigate the latitudinal dependence of magnetic field direction, a standard approach in paleomagnetism is to calculate the geocentric dipole that would give rise to the observed site directions, where the VGP is the position that the dipole pierces Earth’s surface (cf. Butler, 1992). Here we use the paleomagnetic definition of sites, which are assumed to capture individual snapshots of the magnetic field, i.e., a single cooling unit. The dispersion about a mean pole $S$, from a set of $n$ VGPs contained in a locality or latitude band, can then be determined as an estimate of paleosecular variation, where

$$S = \left[ \frac{1}{n-1} \sum_{i=1}^{n} \Delta_{i}^2 \right]^{\frac{1}{2}}. \quad (5)$$

Here, $\Delta_{i}$ is the angular distance of the $i$th VGP from the geographic pole or mean VGP. Note, for paleomagnetic data, $S$ would further be corrected to remove within site dispersion due to random errors in measuring and sampling (e.g., Cromwell et al., 2018).

It has been observed that $S$ varies as a function of latitude, for which various explanations have been hypothesized (cf. Merrill et al., 1996). The phenomenological Model G of McFadden et al. (1988) is often used to approximate the latitudinal variation of VGP dispersion where $S$ is described as a function of (paleo)latitude and two parameters, $a$ and $b$,

$$S^2 = a^2 + (b\lambda)^2. \quad (6)$$

Here, $a$ and $b$ are argued to represent variations in the equatorially symmetric and equatorially anti-symmetric spherical harmonic decomposition of the field, respectively. The $a$ and $b$ parameters are calculated by a least squares fit between the measured VGP dispersion curve and that determined by Model G.
For our criteria we have chosen to apply the quadratic fit, as defined by Model G, as a metric of PSV behavior, with $a$ and $b$ parameters defining separate criteria ($\text{VGP}_a$ and $\text{VGP}_b$). We treat the compliance with the minimum (equatorial) dispersion, $a$, and the latitude dependence, $b$, separately in our framework, since these characterize different aspects of field variability.

The input simulated data for VGP dispersion are $S$ values calculated after using a Vandamme cutoff for both Earth data and simulated outputs ($S_{V_D}$; Vandamme, 1994). The Vandamme cutoff helps to exclude anomalous VGP data, with the intention of preventing bias in the dispersion estimate from magnetic excursions or reversals. The Vandamme cutoff is not constant, but instead is allowed to vary as follows

$$\lambda_{cut} = 90^\circ - (1.8S + 5^\circ), \quad (7)$$

where $S$ is calculated from the simulated data. Sites with VGP latitudes less than $\lambda_{cut}$ are excluded, $S$ is recomputed, and the procedure is repeated until all remaining VGPs are within the cutoff angle. The final $S$ value is then noted as $S_{V_D}$.

Like magnetic directions, the intensity of the magnetic field is also latitudinally dependent. To remove this dependence, a VDM is calculated, which is the strength of the geocentric dipole that produces the observed field intensity $F$, at a given paleolatitude

$$VDM = \frac{4\pi r_e^3}{\mu_0} F (1 + 3 \cos^2 \theta_m)^{-\frac{1}{2}}, \quad (8)$$

where $r_e$ is radius of Earth’s surface, $\theta_m$ is the magnetic colatitude calculated using the mean inclination and the axial dipole equation (1), and $\mu_0$ is the permeability of free space.

To provide an estimate of temporal variation in magnetic intensity, in this study we chose to measure the variability of a distribution of VDMs ($\text{VDMVar}$), through

$$V\% = \frac{\overline{VDM}}{V\overline{DM}_{med}}, \quad (9)$$
where $V_{DM}$ is the interquartile range of a distribution of VDM values, and $V_{DM_{med}}$ is the corresponding median. The VDMVar criterion is passed if the $V\%$ calculated from simulated data falls within the range estimated for Earth.

2.1.3 Criteria Based on Other Paleomagnetic Observables

The final criterion assesses dipole field reversals ($Rev$). The $Rev$ criterion is met if a simulation reverses in an Earth-like manner. While reversals are a fundamental feature of Earth’s magnetic field, an agreed formal description remains elusive. Here, we define a set of standards that we think faithfully represent the fundamental characteristics of geomagnetic field reversals. To pass this criterion a simulation must: a) exhibit at least one reversal in the dipole field after the initial transient period, b) result in a new stable direction, and c) the proportion of time spent in a transitional state is within the range calculated for Earth. For our simulations, we estimated the first two standards by first calculating $\tau_n$, the relative proportion of time spent with a normal polarity (i.e., the time spent with true dipole latitudes $>45^\circ$ divided by the total simulation time), $\tau_r$, the relative proportion of time with a reverse polarity (i.e. the time spent with true dipole latitudes $<45^\circ$ divided by the total simulation time), and $\tau_t$, the relative proportion of time spent in transitional periods (i.e. the time spent with true dipole latitudes between $45^\circ$ and $-45^\circ$ divided by the total simulation time). A simulation passes the first two requirements if both $\tau_n$ and $\tau_r$ are greater than $\tau_t$. Finally, if the calculated $\tau_t$ for a simulation falls within the range estimated for Earth, the simulation passes the $Rev$ criterion.

2.2 Acceptance Thresholds Based on Earth Values for the Past 10 Myr

Establishing acceptance thresholds for $Q_{PM}$ criteria that are representative of Earth’s long-term magnetic field behavior is non-trivial. Ideally, the values for the established criteria
should be representative of the paleomagnetic field for all of Earth’s history. However, it has been hypothesized that PSV and the TAF structure are dependent on conditions at the core-mantle boundary (CMB), and therefore are expected to be variable throughout geologic time (Jones et al., 1977). For the purpose of this study, we consequently chose to focus on the PSV and TAF structure of the paleomagnetic field for the last 10 Myr. This time period was chosen because paleomagnetic data for the last 10 Myr provide sufficient temporal and spatial coverage to enable global analysis, and are additionally young enough to not be strongly affected by plate motion and changing CMB conditions. For the assessment of TAF and PSV behavior for the past 10 Myr we utilized two datasets, PSV10 (Cromwell et al., 2018) and the PINT database (Biggin et al., 2009). For an assessment of reversal behavior for Earth for the past 10 Myr we utilized the 2012 Geomagnetic Polarity timescale (Ogg, 2012). Acceptance thresholds based on Earth values for our chosen criteria as measured are reported in Table 1. A description of the datasets and how specific criteria were estimated is presented in the Supplementary materials.

2.3 Rating Compliance with the Paleomagnetic Field

To rate the compliance of the numerical simulation output with long-term magnetic field behavior we first define a misfit parameter for each criterion, $\Delta Q_{PM}^i$, where $i$ denotes the five criteria VGPa, VGPb, Rev, VDMVar, and IncAnom. We chose to use this method because it is non-parametric, as the distribution of paleomagnetic data is not well-constrained. Here, $\Delta Q_{PM}^i$ is calculated by

$$\Delta Q_{PM}^i = \frac{|m_{Earth}^i - m_{Sim}^i|}{\sigma_{Earth}^i + \sigma_{Sim}^i}.$$  (10)

This parameter is the ratio of the absolute distance between the median Earth value ($m_{Earth}^i$) for a given criterion, $i$, and the median value estimated from the simulated data ($m_{Sim}^i$)
to the total distance covered by the uncertainty bounds (measured as 95% confidence intervals)
that lie between Earth and the simulated data \((\sigma_{Earth}^l + \sigma_{Sim}^l)\). E.g., if \(|m_{Earth}^l| > |m_{Sim}^l|\), then
\(\sigma_{Earth}^l\) would be the lower 95% confidence bound for Earth and \(\sigma_{Sim}^l\) would be the upper 95%
confidence bound for the simulated data, and vice versa when \(|m_{Earth}^l| < |m_{Sim}^l|\). If \(\Delta Q_{PM}^l \leq 1\),
then the simulation passes the criterion and the \(Q_{PM}^l\) score for that criterion is set to 1, otherwise
the \(Q_{PM}^l\) score is set to 0.

Once each criterion is assessed, the total misfit \(\Delta Q_{PM}\) and the total \(Q_{PM}\) score can be
calculated as

\[
\Delta Q_{PM} = \sum_{i=1}^{5} \Delta Q_{PM}^l. \quad (11)
\]

and

\[
Q_{PM} = \sum_{i=1}^{5} Q_{PM}^l, \quad (12)
\]
respectively. If \(\Delta Q_{PM} \leq 5\) and \(Q_{PM} = 5\), then a simulation meets all set criteria.

3. Methods

3.1 Geodynamo Simulations

The geodynamo simulations parametrization and solution methods used in this study
have been extensively documented elsewhere (Davies and Constable, 2014; Davies and Gubbins,
2011; Willis et al., 2007) and so only a brief description is given here. An incompressible
Boussinesq fluid is confined within a spherical shell of width \(d = r_o - r_i\), where \(r_i\) and \(r_o\) are the
inner and outer boundary radii respectively, rotating about the vertical direction at an angular
frequency \(\Omega\). The system is thermally driven and the Boussinesq approximation is employed so
that density variations are accounted for only in the buoyancy force. The fluid has a constant
kinematic viscosity \(\nu\), thermal diffusivity \(\kappa\), thermal expansivity \(\alpha\), and magnetic diffusivity \(\eta\) =
\( (\sigma \mu_0)^{-1} \), where \( \sigma \) is the electrically conductivity. The shell aspect ratio is fixed to \( \eta / r_o = 0.35 \) in this study and Prandtl number \( (Pr = \frac{\nu}{\kappa}) \) is set to 1. The following parameters control the system;

\[
E = \frac{\nu}{2 \mu d^2}, \tag{13}
\]

\[
Pm = \frac{\nu}{\eta}, \tag{14}
\]

\[
Ra = \frac{ag\beta a^2}{2\Omega \kappa}. \tag{15}
\]

Here, \( g \) is gravity, \( Ra \) is the modified Rayleigh number, and \( \beta / d \) is the amplitude of the prescribed temperature gradient at the outer boundary. The solution consists of the magnetic field \( B \), fluid velocity \( u \), and temperature \( T \) throughout the spherical shell and at each time point.

All simulations employ no-slip boundary conditions, that is \( u = 0 \) at \( r_i \) and \( r_o \). For the magnetic field, the top and bottom boundaries are insulating. Therefore, above the core region the magnetic field is represented by a potential field that matches to the dynamo solution at \( r_o \).

Fixed heat flux is prescribed at \( r_o \) in all simulations (denoted FF), while FF or fixed temperature (FT) conditions are applied at \( r_i \). Some simulations additionally employ lateral variations in heat flow at \( r_o \). Here the pattern is either derived from the seismic shear-wave velocity model of Masters et al. (1996) or a recumbent \( Y_2^0 \) heat flux pattern is used as an approximation to the observed shear-wave structures (Dziewonski et al., 2010). The amplitude of the heat flow anomalies is defined by the parameter \( \epsilon = (q^{max} - q^{min})/q^{ave} \), where \( q^{max} \), \( q^{min} \) and \( q^{ave} \) are the maximum, minimum and average heat flow on the outer boundary. We consider values of \( \epsilon = 0.3 - 1.5 \) (Table 2) and note that the largest values do not conflict with the Boussinesq approximation (see Mound and Davies, 2017).

In our suite of simulations, 10 have been reported in previous studies (Davies et al., 2008; Davies and Constable, 2014; Davies and Gubbins, 2011; Gubbins et al., 2007) (Table 2). Three
of these simulations were integrated further here [Model 2 (B2), Model 3 (B4), Model 8 (B3)] in addition to 36 new simulations. The parameter regime explored in these simulations is as follows: $E = 10^{-3} - 1.2 \times 10^{-4}$, Rayleigh numbers ranging from 20-450 corresponding to roughly 1-100 times the critical value for onset of non-magnetic convection, and magnetic Prandtl numbers ranging between 2 and 20 (Table 2). All simulations were run for ~3-30 outer core magnetic diffusion times, or the equivalent of a minimum of about 300 kyr – 3 Myr using the electrical conductivity value of $3 \times 10^5$ S/m from Stacey and Loper (2007).

### 3.2 $Q_{PM}$ Criteria Calculation Protocol

For the assessment of $Q_{PM}$ criteria, Gauss coefficients up to spherical harmonic degree $l_{max}=10$ were calculated at Earth’s surface for each simulation. From the truncated data, we generated simulated values of declination ($D$), inclination ($I$), and intensity ($F$) using a spherical harmonic expansion, where $V$ is the magnetic scalar potential and $\mathbf{B} = -\nabla V$, defined according to

$$V(r, \theta, \phi) = r_e \sum_{l=1}^{l_{max}} \sum_{m=0}^{l} \left( \frac{r_e}{r} \right)^{l+1} (g_l^m \cos m\phi + h_l^m \sin m\phi) P_l^m (\cos \theta), \quad (16)$$

$$I = \tan^{-1} \left( \frac{-B_r}{(B_\theta^2 + B_\phi^2)^{1/2}} \right), \quad (17)$$

$$D = \tan^{-1} \left( \frac{B_\phi}{-B_\theta} \right), \quad (18)$$

$$F = \sqrt{B_r^2 + B_\theta^2 + B_\phi^2}. \quad (19)$$

Here, $r$, $\theta$, and $\phi$ are spherical coordinates (radius, colatitude, and longitude), $P_l^m$ are the Schmidt-normalized associated Legendre functions of degree $l$ and order $m$, and $g_l^m$ and $h_l^m$ are the Gauss coefficients.
For the assessment of PSV and the TAF behavior, we chose to downsample our simulations to mimic the spatial and temporal coverage of real data present within PSV10, thereby mitigating against potential biases due to uneven spatial and temporal sampling. To do this, simulations were downsampled to each of the 51 modified PSV10 localities (see Supplementary materials, Table S1). At each locality, $N$ random time-steps were chosen from the simulation, where $N$ is equal to the number of sites at that locality. Values for $D$, $I$, $F$, VGP latitude, VGP longitude, and $VDM$ for that time-step at that locality were then calculated as per standard paleomagnetic methods (Eqns. 16-19 and 8, respectively, for VGP latitude and longitude see Butler, 1992). Simulated data were normalized to the same polarity. From these parameters, $\Delta I$, $a$, $b$, and $V\%$ were calculated as described in section 2. To address the potential for statistical variation we repeated the downsampling procedure 10,000 times, from which 95% confidence intervals were estimated for each calculated parameter.

4. Results

In our Q$_{PM}$ assessment of 46 geodynamo simulations we find that no simulation successfully reproduces all observed features of the paleomagnetic field. Total $Q_{PM}$ scores for the 46 geodynamo simulations are in the range from 0 to 3, out of a maximum score of five, with a median score of 1 (Fig. 1a). The VGPb criterion had the highest pass rate of 63%, followed by the IncAnom criterion at 35%, VDMVar at 20%, VGPa at 7%, and ending with Rev at 4% (Fig. 1b). Of the 46 simulations assessed, 22 reversed, but only two had $\tau_i$ values within the range for Earth, thus passing Rev. The VGPa criterion was only met by three simulations (Fig. 1b), and none of these simulations reversed (Table 3). Of the four simulations that had $Q_{PM} = 3$, all passed VGPb and IncAnom, three passed VDMVar, one passed Rev, and none passed VGPa.
Representative examples of simulations that pass or fail each criterion are presented in Fig. 2 (Rev), Fig. 3 (IncAnom), Fig. 4 (VGPa and VGPb), and Fig. 5 (VDMVar). All assessed simulation results are presented in Supplemental Figures S1-3. Values for all calculated $Q_{PM}$ parameters are given in Supplemental Table S2 and $Q_{PM}$ results are in Table 3.

Total misfit values, $\Delta Q_{PM}$, for all 46 simulations range from 5.6 to 22.2, with a median value of 10.5. VGPa had the highest median misfit value of 3.4 (Fig. 1c). In a majority (74%) of simulations, misfit values for VGPa were higher than for any other criterion (Fig. 1c). The distribution of $\Delta Q_{PM}$ reveals no correlation between total $Q_{PM}$ score and $\Delta Q_{PM}$ (Fig. 1d). This lack of correlation clearly highlights that none of our simulations are simultaneously reproducing all aspects of Earth’s long-term field behaviour; if a simulation is reproducing some aspects of the paleomagnetic field behavior (highlighted by $Q_{PM}$ scores of 2 or 3), often it is very far from reproducing a different aspect (evidenced by high $\Delta Q_{PM}$ values). In the majority of cases with high $Q_{PM}$ scores and high $\Delta Q_{PM}$ (74%), the parameter with the highest misfit ($\gg 1$) is VGPa.

The distributions of simulated values for each $Q_{PM}$ criterion generally display two peaks that fall to either side of Earth values for the last 10 Myr (Fig. 6). For most criteria, the simulations fail to pass because simulated values were higher than Earth (except for VGPb, where the latitude dependence of VGP dispersion is equally under or over represented relative to Earth). Furthermore, for each criterion, simulations showing reversals had higher simulated values than those that did not reverse, with the highest values obtained for simulations with $\tau_r > 0.15$. Reversing simulations show high VGP dispersion and $\Delta I$, but Earth-like $V\%$ values. In general, non-reversing simulations have lower VGP dispersion and high $\Delta I$, and often insufficient variation in field strength to pass the VDMVar criterion (Fig. 6). No reversing simulations passed the VGPa criterion, with calculated values higher than those observed for
Earth (Fig. 6). In general, positive correlations are observed between calculated values for $V\% - \Delta I$, $V\% - b$, $a - b$, $\tau_t - a$, and $\Delta I - a$ (Supp Fig. S4), forming a quasi-linear trend that contains Earth.

No universal trends between $Q_{PM}$ or $\Delta Q_{PM}$ and input parameters for the simulations assessed in this study were identified. In general, the application of inhomogeneous boundary conditions pushed simulations further from Earth, as reflected in increased $\Delta Q_{PM}$ values as $\epsilon$ increases (Table 3). However, this trend only applies when the application of an inhomogeneous boundary condition resulted in a reversing simulation with $\tau_t > 0.15$. In the case where a simulation with an inhomogeneous boundary condition remained non-reversing, there are small changes in the calculated parameters (Table S2), which results in a lower misfit score with increasing $\epsilon$. Future work will need to be conducted to further determine the effects of heterogeneous boundary conditions on long-term field behavior. In general, there is a positive trend between the magnetic Reynolds number ($Rm = Ud/\eta$, where $U$ is the time-averaged RMS flow amplitude) and all calculated parameters utilized for $Q_{PM}$ assessment (Supp. Fig. S5).

Plotting our simulation results as a function of magnetic Ekman number ($E_\eta = E/Pm$) and $Rm$ shows that many of our simulations fall within the wedge-shaped region of Christensen et al. (2010) for simulations with FF boundary conditions (Fig. 7). However, conformance with Earth’s long-term field behavior for simulations that fall within the wedge is not assured as $Q_{PM}$ scores within the wedge range from 0 to 3 and $\Delta Q_{PM}$ values range from ~6 to 22. Furthermore, many of our simulations that performed relatively well, with $\Delta Q_{PM}$ less than 10, fall outside of the wedge.

5. Discussion
5.1. Limitations of QPM Approach

One limitation of the presented QPM criteria is that only data from the past 10 Myr are used to calculate values for Earth’s TAF and PSV behavior and are not necessarily representative of all periods of Earth history. As stated previously, we utilize paleomagnetic records for the past 10 Myr because this time period represents the most comprehensive record of TAF and PSV behavior. However, the QPM framework can be used for any interval of Earth history where a sufficient quantity of robust paleomagnetic data are available, but the relative importance of each criterion and associated acceptance regions will need to be updated to reflect paleomagnetic behavior for that time period. We also acknowledge, as discussed in section 2, that alternative paleomagnetic observables exist which are not used here. Notwithstanding, the parameters chosen for QPM criteria are based on well-established and commonly employed measures in paleomagnetic studies. We are confident that they appropriately describe the paleomagnetic field and are suitable to assess the degree to which geodynamo simulations are accurately replicating Earth’s long-term magnetic field behavior.

A caveat to the QPM framework, and to any other study that uses the observed field to assess dynamo simulations, is that reproducing these paleomagnetic observables does not inherently demonstrate that a simulation is Earth-like. Magnetohydrodynamic theory suggests that the magnetic, Coriolis and buoyancy (Archimedian) forces are dominant in the momentum equation, termed MAC balance (e.g. Aubert et al., 2017; Starchenko and Jones, 2002). However, it is currently unclear whether the core is in a global MAC balance (Aurnou and King, 2017) and the issue cannot be resolved by current observations. It appears that MAC balance emerges in simulations as $E$ and $P_m$ are reduced towards geophysically relevant values (Aubert et al., 2017; Schaeffer et al., 2017), though some simulations at relatively high $E(\sim 10^{-4})$ may display MAC
balance at leading order with non-negligible secondary contributions from viscous and inertial effects (Aubert et al., 2017; Dormy, 2016). As stated previously, low $E$ and $Pm$ values have not been achieved in simulations that span long timescales. In view of these limitations, here we chose to focus on criteria that can be derived from paleomagnetic observations and do not consider those based on the internal dynamics of the simulations.

5.2 Implications of Simulation Assessment

An unexpected outcome from our assessment of 46 simulations using the QPM criteria is that none are simultaneously reproducing all aspects of Earth’s paleomagnetic field and that there are no obvious combinations of control parameters which will yield a simulation that reproduces Earth’s long-term field behavior. This result contrasts with the findings in Christensen et al. (2010), who showed that geodynamo simulations within a certain $E_{\eta}/Rm$ space can reproduce properties of the historical field. A potential explanation for the discrepancy between our results and those of Christensen et al. (2010) is that the uncertainty estimated for Earth parameters in the two studies were constructed following different approaches. Because the different time-dependent models of magnetic observations utilize direct and indirect observations, and span different time intervals, Christensen et al. (2010) assigned generalized 1-σ error bounds ranging from a factor of 1.75 - 2.5 times the magnitude of the observation to their Earth parameters. For our criteria, we instead utilized 95% confidence bounds calculated directly from paleomagnetic data. Our most restrictive criterion is VGPa, but it is arguably one of the best constrained Earth parameters for the last 10 Myr. The determination of $a$ is dependent upon $S_{VPD}$ values for localities near the equator. In the PSV10 dataset, there are eight localities with latitudes between 10° and -10° ranging across all longitudes, with a
minimum number of sites at each locality of at least 33. The maximum $S_{VD}$ values estimated from these localities is $\sim 15^\circ$ (including 95% confidence intervals) and the minimum is $\sim 6^\circ$, which is the absolute range that $a$ can fall within. Even if we use these estimates for our range for Earth $a$ values, our simulations are still well outside this range with a minimum $a$ value of $\sim 27^\circ$ for simulations that reverse. Furthermore, a recent compilation of directional data for the Cretaceous and Middle Jurassic suggests that $a$ values were between $\sim 8^\circ$ and $13^\circ$ for these time periods, respectively, similar to our estimates for the past 10 Myr (Doubrovine et al., 2019). If we use the same approach as Christensen et al. (2010) for estimating uncertainty bounds, it would extend the values for $a$ from $0^\circ$ to $36^\circ$, at 1σ; such a range is inconsistent with estimates determined by paleomagnetic data.

An additional potential cause of the discrepancy between our findings and those of Christensen et al. (2010) could simply be that the field morphology observed for the historical field is not the one expected for long time scales and that secular variation of the recent field does not accurately reflect the behavior of the long-term paleomagnetic field. This is quite plausible given that spontaneous variations in field behaviour appear, from e.g. the PADM2M dipole model (Ziegler et al., 2011), to be active on timescales far longer than those captured in time-dependent field models.

The relatively low total $Q_{PM}$ scores achieved by our simulations appears to be related to a tendency for many simulations (particularly those which reverse) to produce strong and/or strongly variable non-$g_1^0$ components. Generally, simulations that reverse have higher $\Delta l$, $a$, $b$, and $V\%$ values (falling significantly outside the range of Earth), suggesting that these high/more variable non-$g_1^0$ components are more prevalent in reversing and multipolar simulations, as known from previous dynamo studies (Christensen and Aubert, 2006; Kutzner and Christensen,
This trend may not hold true for all reversing simulations, as only two simulations passed Rev in this study, and more simulations should be assessed in the future to test this trend. To find a simulation that better captures Earth’s paleomagnetic field, the non-$g_{10}$ components must be reduced while the $g_{10}$ term remains capable of spontaneously changing its sign. Simulations that reverse and maintain a larger degree of dipole dominance have been produced in previous studies (e.g., Driscoll and Olson, 2009; Lhuillier et al., 2013; Wicht et al., 2009; Wicht and Meduri, 2016) and in future work it would be valuable to assess how these simulations perform using the $Q_{PM}$ criteria. In our study, the only simulations with $\Delta Q_{PM}$ values approaching the Earth-like regime are those that do not reverse, suggesting that we currently cannot exclude non-reversing simulations in our quest for an Earth-like simulation.

We can conclude that simulations which fall within the ‘wedge’ of Christensen et al. (2010) are not guaranteed to reproduce Earth’s paleomagnetic field behavior, and that compliance with the long-term magnetic field should be assessed separately, similar to findings of Davies and Constable (2014) for the Holocene. This is especially pertinent for studies that use the output from numerical geodynamo simulations to formulate corrections to paleomagnetic data [e.g., Driscoll and Wilson (2018), Lhuillier and Gilder (2013)], as these corrections may include non-Earth-like TAF and PSV behavior.

In this study we did not find long-duration simulations which simultaneously reproduce all aspects of Earth’s paleomagnetic field behavior. However, our exploration of the possible parameter space is not exhaustive, and the fact that our simulations bracket Earth values suggest that a simulation reproducing Earth’s paleo-field behavior should exist within a computationally accessible parameter regime. Overall, more long-duration simulations need to be assessed using the $Q_{PM}$ criteria in the future.
6. Conclusions

We developed a framework for assessing the compliance between numerical geodynamo simulations and long-term magnetic field behavior ($Q_{PM}$ criteria). Using $Q_{PM}$ criteria, the compliance of 46 simulations with magnetic field behavior for the past 10 Myr was considered. We found that our simulations achieved a maximum $Q_{PM}$ score of 3 out of 5, with most simulations scoring much lower, and with median $\Delta Q_{PM}$ misfit values of ~10, where less than 5 indicates compliance with Earth behavior. Low $Q_{PM}$ scores appear to be partly due to enhanced non-$g_1^0$ components relative to those observed for the last 10 Myr on Earth. There appears to be no specific combination of $E_{\eta}/Rm$ parameters in which simulations reliably replicate Earth’s long-term field behavior. Furthermore, we find that compliance with the criteria set by Christensen et al. (2010) does not guarantee that a simulation reproduces Earth-like TAF and PSV behavior.

The $Q_{PM}$ framework can provide a path towards developing simulations which can reproduce Earth’s long-term magnetic field behavior in the future. This framework can be modified to represent periods of different geodynamo behavior in Earth’s past, e.g. the Cretaceous or Middle Jurassic, allowing for a more robust characterization of the evolution of the deep interior through Earth’s history, provided a sufficient quantity of robust paleomagnetic data are available.

Acknowledgements

CJS, AJB, and CJD acknowledge support from the Natural Environment research council (standard grant, NE/P00170X/1); AJB, RKB, and DGM acknowledge support from The
Leverhulme Trust (Research Leadership Award, RL-2016-080); CJD acknowledges a Natural Environment Research Council personal fellowship, reference NE/H01571X/1. A portion of the geodynamo simulations were performed on the UK National service ARCHER (via allocation through the Mineral Physics Consortium). We would like to thank Hagay Amit for his constructive and thorough reviews which helped improve this manuscript.

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Figure Captions:

Figure 1. A. Bar graph showing the number of simulations that received scores of 0, 1, 2, and 3, respectively. Note, no simulation received $Q_{PM}$ scores of 4 or 5. B. Bar graph showing the number of simulations that passed (failed) in blue (red) for each criterion. The percentage marks the percent of simulations that passed. C. Box plot of $\Delta Q_{PM}$ values over all simulations for each criterion. Horizontal lines mark median values, boxes outline the interquartile range (IQR), and error bars show full range excluding outliers (diamonds) which are defined as being more than 1.51 IQR outside the box. The dashed line indicates a target value of 1, and data below this line pass the respective criterion. D. Histogram of $\Delta Q_{PM}$ values for all simulations. Colors within each $\Delta Q_{PM}$ bin indicate total $Q_{PM}$ score. For color see online version.

Figure 2. Representative reversal behavior for three end-member behaviors observed from the evaluated simulations: 1) Simulations that failed to reverse, 2) Simulations that passed the Rev criterion, and 3) Simulations that reversed but had $\tau_t > 0.15$ and failed Rev. In each subplot, the
Figure plots calculated true dipole latitude versus time in years, calculated using the diffusion timescale and the electrical conductivity value of $3 \times 10^5$ S/m from Stacey and Loper (2007). Dipole latitude is reported in degrees.

Figure 3. Representative $\Delta I$ vs. latitude curves showing three end-member behaviors observed from the evaluated simulations: 1) Simulations that failed the IncAnom criterion due to low values, 2) Simulations that passed the IncAnom criterion, and 3) Simulations that failed the IncAnom criterion because values were too high. In each plot, data points mark the median $\Delta I$ values and 95% confidence bounds estimated from the repeated 10,000 downsampling routines, for each $10^\circ$ latitude band. The star indicates the maximum median $\Delta I$ value used to evaluate the $Q_{PM}$ criterion. The dashed blue lines mark the 95% confidence bounds for Earth and the negative equivalent. Units are in degrees.

Figure 4. Representative VGP dispersion (using the Vandamme cutoff) vs. latitude curves for four end-members behaviors observed in the evaluated simulations: 1) Simulations that failed because $a$ was too high but $b$ passed, 2) Simulations that passed both VGPa and VGPb, 3) Simulations that failed because both $a$ and $b$ values were too high, and 4) Simulations that failed because both $a$ and $b$ values were too low. The red solid line marks the Model G curve plotted using median $a$ and $b$ parameters and the light red envelope marks the 95% confidence interval. The solid blue line in each figure is the Model G curve calculated from median $a$ and $b$ parameters for Earth and the light blue envelope marks the 95% confidence interval (for color see online version). Units are in degrees.
Figure 5. A. Representative $V\%$ values and dipole moment distributions (calculated without downsampling, units are non-dimensionalized) for three end-member behaviors observed from the evaluated simulations: Model 30) Simulation that failed because the $V\%$ value was too low, Model 6) Simulation that passed, and Model 1) Simulation that failed because the $V\%$ value was too high. The dashed lines in A mark Earth range. Insets plot the distribution of virtual dipole moments for Earth between 0-1 Myr (B) and 1-10 Myr (C), units are in ZAm$^2$ ($10^{21}$).

Figure 6. Histograms of calculated values from each simulation, shown for each criterion, colored by the proportion of data from simulations that are in the locked regime of convection (lock e.g. Davies et al., 2008; light blue), did not reverse (Non; blue), reversed (Rev; dark blue), and reversed but had $\tau_t > 0.15$ and did not pass Rev (MP; darkest blue). Pink boxes mark the range for Earth values in each subplot. For color see online version.

Figure 7. Evaluated dynamo simulations plotted as a function of magnetic Ekman number ($E_\eta$) vs. Magnetic Reynolds number ($Rm$) following Christensen et al. (2010). Circle size denotes total $Q_{PM}$ score, with the largest circles having scores of 3 and the smallest circles having scores of 0. Color denotes total misfit value, $\Delta Q_{PM}$. The dashed line marks the wedge-shaped region that contain simulations with Earth-like misfit scores ($\chi^2 < 4$) and FF boundary conditions in Christensen et al. (2010).

Table 1. Summary of Earth time average field and paleosecular variation values. Med indicates median values, high indicates the upper 95% confidence bound, and low indicates lower 95% confidence bound. Values for $a$, $b$, and $\Delta I$ were calculated from data presented in Cromwell et
al. (2018), $V\%$ values for the 0-1 Ma interval and 1-10 Ma interval were calculated from data presented within the PINT15 database, and $\tau_t$ values were estimated from Ogg (2012).

Table 2. Summary of input and output parameters for assessed geodynamo simulations. Sim. Name = Simulation Name, $Pr$ = Prandtl number, $Pm$ = Magnetic Prandtl number, $E$ = Ekman number, $Ra$ = Rayleigh number, $\varepsilon$ = amplitude of prescribed outer boundary heat flux heterogeneity, BC = boundary condition (inner-outer), $Rm$ = Magnetic Reynolds number, and Rev indicates reversing regime defined using $\tau_t$. non=non-reversing, rev=reversing with $0.0375<\tau_t<0.15$, and multi= $\tau_t>0.15$. Note, parentheses in Sim. Name indicate previously published or further integrated simulations, where the name in parentheses corresponds to the name used in Davies and Constable (2014). * indicate simulations that utilized an inhomogeneous boundary condition after Masters et al. (1996). Unless noted, all other inhomogeneous boundary conditions utilized a recumbent $Y_2^0$ heat flux pattern (Dziewonski et al., 2010).

Table 3. Summary of $\Delta Q_{PM}$ and $Q_{PM}$ scores for assessed geodynamo simulations. Rev indicates reversing regime as defined in Table 2. Sim. Name = simulation name (see Table 2 caption for details), $\tau_t$ = proportion transitional, $\Delta Q_{PM}$ = $\Delta Q_{PM}^i$ misfit values for each respective criterion, and $Q_{PM}$ = $Q_{PM}^i$ score for each respective criterion.