Mildly Hierarchical Triple Dynamics and Applications to the Outer Solar System

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Abstract

Three-body interactions are ubiquitous in astrophysics. For instance, Kozai–Lidov oscillations in hierarchical triple systems have been studied extensively and applied to a wide range of astrophysical systems. However, mildly hierarchical triples also play an important role, but they are less explored. In this work, we consider the secular dynamics of a test particle in a mildly hierarchical configuration. We find the limit within which the secular approximation is reliable when the outer perturber is in a circular orbit. In addition, we present resonances and chaotic regions using surface-of-section plots, and characterize regions of phase space that allow large eccentricity and inclination variations. Finally, we apply the secular results to the outer Solar System. We focus on the distribution of extreme trans-Neptunian objects (eTNOs) under the perturbation of a possible outer planet (Planet 9), and find that in addition to a low-inclination Planet 9, a polar or a counter-orbiting one could also produce pericenter clustering of eTNOs, while the polar one leads to a wider spread of eTNO inclinations.

Unified Astronomy Thesaurus concepts: Three-body problem (1695); Solar system (1528); Trans-Neptunian objects (1705); Celestial mechanics (211)

1. Introduction

The three-body problem is one of the oldest problems in astrophysics. Due to its chaotic nature, no general solution is possible; however, important results can be obtained using perturbative approaches. For instance, when one of the objects is much farther from the other two objects (in a hierarchical configuration), one can treat the influence of the farther object as a weak perturbation and discover interesting dynamical properties. Kozai (1962) and Lidov (1962) developed the framework to study such three-body systems. It was found that, when the members of the inner binary (composed of the two closely separated objects) are inclined ($i_{\text{in}} > 40^\circ$) with respect to the orbit of the farther object (outer orbit), Kozai–Lidov resonances could lead to large-amplitude eccentricity and inclination variations of the inner binary.

Due to the prevalence of three-body systems in hierarchical configurations, the Kozai–Lidov mechanism has since been applied to explain a wide variety of astrophysical phenomena. Inspired by the objects in our Solar System, the Kozai–Lidov mechanism focused on systems with a circular outer orbit. In this case, expanding the disturbing function to second order in the small parameter (semimajor axis ratio of the inner and outer orbit, $a_1/a_2$) is sufficient. However, the quadrupole limit cannot describe the dynamics when the perturber is eccentric (e.g., Naoz et al. 2011, 2013; Katz et al. 2011), and the disturbing function needs to be expanded up to the octupole order ($a_1/a_2)^3\). With an eccentric outer perturber, the eccentricity of the inner orbit can be excited close to unity. In addition, the inclination of the inner orbit can cross 90°, even when it starts in a near-coplanar configuration with respect to the outer binary (Li et al. 2014b). This can explain a wide range of astrophysical phenomena; for a review, see Naoz (2016).

While the Kozai–Lidov mechanism and the eccentric Kozai–Lidov mechanism mainly describe the evolution of a test particle perturbed by an outer massive object, the evolution of an outer test particle perturbed by an inner binary has also been studied (e.g., Naoz et al. 2017; Vinson & Chiang 2018; de Elía et al. 2019). In contrast to the inner test particle case, the quadrupole resonance allows the outer test particle’s orbit to flip without changing its eccentricity. Higher-order resonances can further excite test particle eccentricity and inclination. This has important implications for the dynamical evolution of debris disks surrounding planets in eccentric orbits (e.g., Zanardi et al. 2017).

Beyond the hierarchical limit, nonhierarchical dynamics also has wide applications but has been explored less. Recently, using a large ensemble of $N$-body simulations, Stone & Leigh (2019) obtained a statistical solution to the chaotic nonhierarchical three-body problem, under the assumption of ergodicity. They found that the nonhierarchical triple interactions almost always lead to a single escaping object and a stable bound binary. In addition, the eccentricity of the surviving binary follows a superthermal distribution.

In mildly hierarchical triples, in which the triple system could still survive, nonsecular effects can become important and can enhance the inner binary eccentricity (e.g., Cuk & Burns 2004; Antonini & Perets 2012; Antonini et al. 2014). In particular, Luo et al. (2016) showed that short-timescale oscillations can accumulate and make the secular results unreliable. They obtained “corrected double averaging” equations to account for the error in the secular results. Based on this correction, Grishin et al. (2018) obtained analytical results on the maximum eccentricity of the inner binary at the quadruple level.

However, the secular results can still provide a good approximation when the perturber is much less massive than the central object, and the corrected terms at the quadruple level are not sufficient when the three objects are closer to each other (with semimajor axis ratio $\geq 0.3$). In particular, Gronchi & Milani (1998) studied the dynamics of near-Earth asteroids, and developed a secular method without expansion of the semimajor axis ratio. More recently, this method has been used to study secular interactions between extreme TNOs and the hypothetical Planet 9 (Beust 2016; Saillenfest et al. 2017; Li et al. 2018). These studies mostly focused on the near-coplanar regime, where Planet 9 is located near the ecliptic plane. Nevertheless, a
systematic study of dynamics of the mildly hierarchical systems is missing from the literature, and the effects of an inclined Planet 9 on the extreme TNOs remain poorly explored.

In this paper, we study the secular interactions in mildly hierarchical systems with either an inner or an outer perturber. We compare the dynamical features to those in the hierarchical limit using a surface-of-section plot, which identifies the location of resonant and chaotic regions. We also identify initial conditions that can lead to large eccentricity and inclination variations. Finally, we apply our results to study interactions between objects in the outer Solar System and the hypothetical Planet 9. The paper is organized the follows. In Section 2, we discuss the numerical techniques we adopt in this work, and in Section 3, we derive the limit where the secular approach is valid. We then present the surface-of-section plots in Section 4, and the maximum eccentricity and inclination variations in Section 5. In Section 6, we apply our results to the objects in the outer Solar System. Finally, we discuss our results and conclude in Section 7.

2. Numerical Methods

Mildly hierarchical triples can be separated into two binaries (as shown in Figure 1). The closely separated two objects, \( m_1 \) and \( m_2 \), form the inner binary, and the outer binary is composed of the farther object, \( m_3 \), orbiting around \( m \). Note that this is different from the generic setup of hierarchical triples, where the outer binary is typically set to originate from the center of mass of the inner binary. This makes little difference here, since the perturbing mass that we consider must be much smaller than the central object for the secular results to be valid.

Here, we use subscript 1 to denote the orbital elements of the inner orbit, and subscript 2 for the outer binary: \( r_1 \) and \( r_2 \) represent the position vectors of \( m_1 \) and \( m_2 \) from the central massive object \( m \). In this paper, we study the dynamics of a test particle in the triple system, and consider configurations with both inner and outer massive perturbers. Thus, depending on the configuration, either \( m_1 \) or \( m_2 \) could be the test particle. We use parameter \( \alpha \) to denote the ratio of the semimajor axis of the test particle with respect to the semimajor axis of the perturber. We set \( \alpha < 1 \) for the inner test particle scenario, and \( \alpha > 1 \) for the outer test particle case. Please note that, in this setup, the choice of reference frame is arbitrary. In test particle approximation, the orbital elements of the perturber are constant and can be used to define the frame of reference. In most of the simulations, we choose a coordinate system in which the inclination \( i_2 \) and longitude of ascending node \( \Omega_2 \) of the perturber are set to be 0.

To describe the motion of a test particle under the influence of the central object and a lower-mass companion, we follow the expressions below (e.g., Murray & Dermott 2000):

\[
\dot{r}_i = \nabla V_{\text{central}} + \nabla R_i, \quad \text{where} \quad V_{\text{central}} = \frac{Gm}{|r|},
\]

\[
R_i = \frac{Gm_j}{|r_j - r_i|} - \frac{Gm_j(r_j, r_i)}{|r_j|^3}.
\]

Here, \( R_i \) is the disturbing function, \( r_i \) and \( r_j \) are the positions of the test particle and the perturber with respect to the central object respectively, \( m_j \) is the mass of the perturber, \( m \) is the mass of the central object, and \( G \) is the universal gravitational constant. The disturbing function describes the interaction potential between the test particle and the perturber as the effect due to the influence of the perturber on the central body. The first term of the disturbing function is called the direct term, and the second one is called the indirect term. Indirect terms do not contribute to secular perturbations, as they average to zero (e.g., Murray & Dermott 2000). We can write the secular disturbing function as

\[
R_{\text{secular},i} = \frac{Gm_j}{4\pi^2} \int \int \frac{1}{|r_i - r_j|} dMdM',
\]

which averages out the fast, orbital timescale variations. In this study, we do not include relativistic effects; rather, we focus only on point-mass Newtonian interactions. We apply our results to the outer Solar System (Section 6), where relativistic corrections are not important.

In the mildly hierarchical limit, the semimajor axis ratio is no longer a small parameter, so we numerically average the disturbing function instead of expanding it in the ratio of semimajor axes. This allows us to explore regimes that are nonhierarchical. Orbital elements of the test particle are evolved using Hamilton’s equations. We use the scale-invariant Delaunay conjugate variables to define our phase space; they are composed of conjugate pairs \( J_3 - \Omega \) and \( J_\omega - \dot{\Omega} \), where in the test particle limit, \( J_3 = \sqrt{1 - e^2} \) and \( J_\omega = \sqrt{1 - e^2} \cos \iota \). The equations of motion are given by:

\[
\dot{\Omega} = -\frac{1}{\sqrt{Gma}} \frac{\partial J_3}{\partial \Omega}, \quad \dot{\iota} = -\frac{1}{\sqrt{Gma}} \frac{\partial J_\omega}{\partial \iota},
\]

\[
\dot{J}_3 = -\frac{1}{\sqrt{Gma}} \frac{\partial J_3}{\partial \iota}, \quad \dot{J}_\omega = -\frac{1}{\sqrt{Gma}} \frac{\partial J_\omega}{\partial \Omega}.
\]

We solve the above set of equations numerically.\(^3\) In nonhierarchical systems, the orbits of the perturber and the test particle can intersect. Although the perturber and the test particle may not actually collide in the unaveraged system, they may coincide at one or more points during the process of averaging. When they do, the disturbing function and its

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\(^3\) The code is publicly available via a git repository hosted at, https://github.com/bhakshar/gla3bd.
derivative have singularities that can be difficult to evaluate. We use the CQUAD integration routine from the GNU Scientific Library (GSL) to perform these integrations. The equations of motion are evolved using GSL’s implementation of the Runge–Kutta–Fehlberg (4, 5) method.

Furthermore, Gronchi & Milani (2001) show that, when orbits cross (or intersect), the derivatives of the disturbing function are not continuous across the crossing. Extra care needs to be taken when orbits cross. Whenever orbits cross during a single time step, we abandon the current step and take a specific time step to land exactly at the intersection. To find the intersection, we use the mutual nodal distance as the independent variable, which allows us to choose a step to reach the intersection (following Henon (1982)). This is similar to the approach used by Saillenfest et al. (2017). Instead of using implicit integration schemes, we use forward (and backward) discrete differentiation to calculate derivatives of the disturbing function from the positive (and negative) direction approaching the intersection separately. This provides the equation of motion prior to (and after) the crossing.

In Figure 2, we show the orbital evolution of a test particle in a hierarchical system (top two panels) and in a mildly hierarchical system (bottom two panels) as calculated by double-averaged simulations (blue), octupole-order simulations (red), and N-body simulations (black). We used the Bulirsch–Stoer integration scheme from the MERCURY simulation package (Chambers & Migliorini 1997) with a time step of 5% of the period of the inner orbit to obtain the N-body results. We show the time in terms of the Kozai timescale given by:

$$t_k = \frac{m_1}{m_2} \left(1 - e_2^2\right)^{3/2} \frac{a_2^3}{a_1^3} P,$$

where $P$ is the orbital period of the inner orbit (e.g., Valtonen & Karttunen 2006). We use the parameter $\epsilon$ to quantify the level of hierarchy:

$$\epsilon = \frac{a_1}{a_2^2} - \frac{e_2}{1 - e_2^2}.$$

The octupole-order disturbing function can accurately describe triple-system dynamics as long as $\epsilon < 0.1$. In hierarchical systems (top), all three methods agree with each other. In nonhierarchical systems (bottom) on the other hand, the octupole-order evolution does not agree with N-body simulations. Meanwhile, double-averaged evolution is in excellent agreement with N-body simulations.

2.1. Comparison to Previous Works

Most studies in the literature rely on the expansions of the disturbing function to study secular evolution in triple systems. Most commonly, the disturbing function is expanded in the eccentricities and inclinations of the interacting particles following the Lagrange–Laplace secular theory (Murray & Dermott 2000). Such expansions have been used to study the interactions between the planets in systems with low eccentricities and inclinations. A special case where the absolute inclinations of the interacting particles are high but the relative inclination are small has also been studied (Boué & Fabrycky 2014). In hierarchical systems, inclination and eccentricity variations can be very high, but the separations between the inner and outer objects are large. Hence, the disturbing function is expanded in the ratio of semimajor axes (Kozai 1962; Harrington 1968). Expansions up to quadrupole, octupole, and hexadecapole-order terms have been explored in detail in the literature (e.g., Yokoyama et al. 2003; Naoz 2016). However, these expansions cannot be used to study nonhierarchical systems where the semimajor axis ratios can be large and orbits can even cross.

Beyond three-body systems, the more general problem of understanding the evolution of large number of interacting particles has also been studied. For instance, Fouvré et al. (2017) study the secular evolution of multiple stars orbiting a black hole using kinetic equations derived from BBGKY hierarchy. Hamers & Portegies Zwart (2016) have developed a method to study the evolution of hierarchical multiple systems composed of nested binaries. This method relies on the expansion of the Hamiltonian in terms of the binary separation ratios. Follow-up studies have included the effects of flybys, instantaneous perturbations (Hamers 2018), and orbit-averaging corrections (Hamers 2020).

Similar to this study, multiple works have used numerical averaging to calculate secular interactions between particles. In particular, Touma et al. (2009) developed the Gaussian ring algorithm, based on the analytical calculation of the orbit-averaged perturbing acceleration due to the force of a softened ring as well as a second average over the perturbed ring itself by numerical quadrature. Applying the Gaussian ring algorithm, Nesvold et al. (2016) modeled the effects of self-gravity in a debris disk by calculating the secular interactions of concentric rings. To include a careful treatment at the point of orbital intersection, our approach closely follows that of Gronchi & Milani (1998), as mentioned above. More recently, this approach has also been used to study the interactions between Planet 9 and extreme trans-Neptunian objects (eTNOs; Beust 2016; Saillenfest et al. 2017).
3. Accuracy of the Secular Results for a Circular, Outer Perturber

The double-averaging method outlined in Section 2 is limited to low-mass perturbers. As the mass of the perturber increases, nonsecular oscillatory effects, such as mean motion resonances and ejection resonances, become important (Luo et al. 2016; Grishin et al. 2018), and the secular approach is no longer reliable. For instance, in the secular regime, the mass of the perturber is just a scaling factor that would only change the dynamical timescale of the system (as shown in Equations (4) and (5)). This is not true when the mass of the perturber is high.

To illustrate this, we perform an ensemble of double-averaged secular simulations and compare them with N-body simulations. We focus on the case of an inner test particle under the perturbation from an object on a circular orbit. We run these simulations for three Kozai timescales (see Equation (6)). To check for consistency, our N-body results were verified with two different integration methods: Bulirsch–Stoer and hybrid integrators of the MERCURY package. In addition, we ran N-body simulations and secular simulations with different time steps (2.5%, 5%, and 10% of the inner orbital period). The fractional differences in $e_{\text{max}}$ of the hybrid integrator do not converge for the different time steps when the eccentricity is high. Thus, we use the Bulirsch–Stoer integrator for our N-body simulations. We find that the results of the secular method and the Bulirsch–Stoer integrator are consistent across different choices of time steps, and the secular results are in excellent agreement with the N-body results (except near mean-motion resonances). The choice of time step did not affect our results as long as the time step for N-body simulations computed using Bulirsch–Stoer integrator was less than ~10% of the period of the innermost object and for secular simulations was less than 0.5% of the secular timescale.

In Figure 3, we plot the maximum eccentricities against the mass of the perturber. The perturber is on a circular orbit, and test particles start on a circular orbit ($e_1 = 0$) with $i_1 = 75^\circ$ and $\Omega_1 = \pi/4$. Three different configurations of the test particle are shown: the panel on the left has a semimajor ratio of $\alpha = 0.1$, the one in the middle corresponds to $\alpha = 0.3$, and the one on the right corresponds to $\alpha = 0.5$. The blue pluses represent the double-averaged results, and the green crosses represent the N-body results. We note that the system becomes chaotic when it gets less hierarchical ($\alpha \gtrsim 0.18$). While the qualitative behavior can still be valid, chaos could affect the specific value of $e_{\text{max}}$ for a certain configuration.

The maximum eccentricity obtained from the double-average results is independent of the perturber’s mass, because the masses only determine the dynamical timescale of the system. For the n-body results, as the mass of the perturber increases, so do the nonsecular effects, causing $e_{\text{max}}$ to increase. A purely secular double-averaging method fails to capture this effect. Thus, as the perturber become more massive, the maximum eccentricity calculated from the double-averaged method ($e_{\text{max}}^{DA}$) starts to deviate from that calculated using N-body simulations ($e_{\text{max}}^{NB}$), as shown in Figure 3.

We use black dashed lines to denote the critical perturber mass, the mass of the perturber above which the double-averaged results start to deviate from the N-body results. Specifically, the critical mass is defined by the following criteria:

$$\frac{\left|\left(1 - e_{\text{max}}^{NB}(m_2)\right) - \left(1 - e_{\text{max}}^{DA}\right)\right|}{1 - e_{\text{max}}^{DA}} > 0.01. \tag{8}$$

As the semimajor axis ratio increases, the nonsecular effects of the perturber become stronger and the critical mass decreases. For low values of $\alpha$, the deviation from the secular results can be explained by single-averaged corrections, which are obtained by averaging the disturbing function only over the orbit of the inner test particle (the shortest timescale in the problem). Luo et al. (2016) derived single-averaged corrections to the double-averaged disturbing function. Using their derivation and the quadrupole-order double-averaged disturbing function, Grishin et al. (2018) derived a single-averaged correction ($\delta e_{\text{core}}^{SA}(m_2, \alpha)$) to $e_{\text{max}}^{DA}$. In Figure 3, red dashed lines represent the results by Grishin et al. (2018). While the quadrupole result agrees very well with N-body results at $\alpha = 0.1$, at higher values of $\alpha$, it fails to agree even for low $m_2$.

Therefore, we use a semi-analytical method that includes terms up to $\alpha^8$ to calculate $\delta e_{\text{core}}^{SA}$, while using the same single
averaged correction \((\delta e^{SA}_{\text{corr}}(m_2, \alpha))\) from Grishin et al. (2018).

By including the eighth order, the semi-analytical approach is a good approximation, using the results of the maximum perturber mass, below which the double average provides a good approximation of eccentricities. When the perturber is on a circular orbit, the Hamiltonian is independent of \(\Omega\), and only terms of even order survive in the Hamiltonian in addition to the single-averaged correction:

\[ H = H_{e=2} + H_{e=4} + H_{e=6} + H_{e=8} + H_{SA}, \]

where the single-averaged correction is derived in Equations (39) of Luo et al. (2016):

\[ H_{SA} = -\frac{27}{8} \epsilon_{SA} \bar{a}_1 \left( \frac{1 - j^2}{3} + 3\epsilon^2 + 5\epsilon^2 \cos(i)^2 \right). \]

\[ \epsilon_{SA} = \left( \frac{a_1}{a_2(1 - e_2^2)} \right)^{3/2} \left( \frac{m_2^2}{(m + m_2)m} \right)^{1/2}. \]

In this case, the maximum eccentricity can be obtained numerically, requiring that energy is conserved:

\[ H(\epsilon = 0, i = i_0, \omega = \pi/2) = H(\epsilon = \epsilon_{SA}^{\text{max}}, i = i_{\text{max}}, \omega = \pi/2). \]

We show the semi-analytical results (cyan lines) in Figure 3. By including the eighth order, the semi-analytical approach agrees very well with the direct N-body simulations at higher values of \(\alpha\) and low values of \(m_2\). However, the semi-analytical results deviate from the N-body results for larger \(m_2\) when \(\alpha \sim 0.5\), suggesting higher-order single-averaged corrections need to be included. Please note that the approach outlined above for the eighth-order expansion works only for a circular perturber. When the perturber is eccentric, the number of degrees of freedom for the system increases to 2 and \(\epsilon_{\text{max}}\) cannot be easily obtained. In addition, wiggles in the numerical results are mainly due to close encounters, which cannot be captured by the secular approach.

In the end, we derive an analytical expression for the critical perturber mass, below which the double average provides a good approximation, using the results of the maximum eccentricities. When the perturber is on a circular orbit, \(j_c\) is a constant of motion as a result of the double average over the inner and outer binary orbits. However, single-averaged corrections lead to oscillations in \(j_c\) with maximum fluctuations proportional to \(\epsilon_{SA}\). Assuming all the deviations between \(\epsilon_{\text{max}}^{DA}\) and \(\epsilon_{\text{max}}\) are due to fluctuations in \(j_c\) and are caused by the single-averaged oscillations, we can obtain the fractional change in the maximum eccentricity due to the single-averaged oscillation effects as the following:

\[ f_e = \frac{\delta \epsilon_{\text{corr}}^{SA}(m_2, \alpha)}{1 - \epsilon_{\text{max}}^{DA}(\alpha)}, \]

where \(f_e = 0.01\) gives the critical mass of \(m_2\) according to our definition in Equations (8), and \(\epsilon_{\text{corr}}^{SA}\) and \(\epsilon_{\text{max}}^{SA}\) in the quadrupole limit are obtained in Grishin et al. (2018) (Equations (33) and (38)).

\[ \delta \epsilon_{\text{corr}}^{SA}(m_2, \alpha) = \frac{135}{128} \epsilon_{\text{max}}^{SA} \epsilon_{SA}^{\text{max}} \left( \frac{16}{9} \right)^{3/5} \left( 1 - \left( \frac{\epsilon_{SA}^{\text{max}}}{\epsilon_{\text{max}}^{SA}} \right)^2 \right), \]

\[ \epsilon_{\text{max}}^{SA} = \sqrt{1 - \frac{5}{3} \cos^2 i_0 \left( 1 + \frac{9}{5} \frac{\epsilon_{SA} \cos i_0}{1 - \frac{9}{5} \epsilon_{SA} \cos i_0} \right)}. \]

To the first order in \(\epsilon_{SA}\) and assuming \(m_2 \ll m\), we can get an analytical expression for the critical mass \(m_{2,\text{crit}}\), where \(f_e < C\):

\[ m_{2,\text{crit}} = \frac{4Cm(6 - \sqrt{6 - 30 \cos(2i_0)})}{15\alpha^{3/2} \cos^2(i_0)(9 - 15 \cos^2(i_0))}. \]

We compare the expression with N-body simulations in Figure 4, which shows the critical mass as a function of \(\alpha\). The dots represent the N-body results, the dashed line represents the analytical results in Equation (16), and the solid red line represents the semi-analytical results based on the eighth-order expansion in semimajor axis ratio \((\alpha_{\text{in}}/\alpha_{\text{out}})^{\alpha}\). When the perturber is close to the test particle \(a_1/a_2 \sim 0.5\), the perturber needs to be small compared with the central object \((\sim 10^{-3.5})\) that of the central object’s mass). When the perturber is farther \((a_1/a_2 \sim 0.1\), the perturber only needs to be lower than \(\sim 10^{-7.5}\) times the mass of the central object for the double average to be valid.

Our analytical expression agrees well with the N-body results when \(\alpha \lesssim 0.3\). When \(\alpha \gtrsim 0.3\), effects of mean motion resonances \((P_1 : P_2 = 1 : 5, 1 : 4, 1 : 3)\) become important, and this makes the analytical results based on the single-averaged method no longer reliable. The semi-analytical results up to the eighth power in \(\alpha\) agree slightly better compared to the analytical expression. When \(\alpha \gtrsim 0.3\), the single-averaged correction becomes similar in magnitude to the expansion at the
n = 8 order (up to $(a_1/a_2)^8$). Thus, one needs even higher-order expansions to obtain more accurate semi-analytical results on the critical mass.

4. Surface-of-section Plots

For systems with perturbing mass much lower than that of the central object ($\sim 10^{-3}$ to $10^{-5}$ m), the secular results using the double-average method provide a good approximation to the dynamics. Thus, to better understand the dynamics of mildly hierarchical triples, we analyze the secular results in this section in more detail. In the test particle limit, the secular dynamics can be reduced to two degrees of freedom, and the phase space is four-dimensional. It is difficult to visualize the phase space directly, and thus we use surface-of-section plots to characterize the dynamical properties, similar to the approach in, e.g., Li et al. (2014a).

We first look at surface-of-section plots in $e \cos \omega - e \sin \omega$ space. We perform an ensemble of secular simulations using the method outlined in Section 2. From the trajectories of the test particles evolved in these simulations, we collect all points on the surface $\Omega = 0$ for inner test particle configurations and $\Omega = \pi/2$ for outer test particle configurations that satisfy the condition $\Omega < 0$. We choose $\Omega = \pi/2$ for the outer test particle configurations because the librating trajectories are centered around $\Omega = \pi/2$ due to the quadrupole resonances (Naoz et al. 2017).

To study how the surfaces change as the system becomes less hierarchical, we make surfaces for different values of the semimajor axes ratio ($\alpha = \{0.1, 0.2, 0.3, 0.5, 2, 3, 5\}$), and we also consider perturbers with different eccentricities ($e_2 = \{0.2, 0.4, 0.6, 0.8\}$). We show a few representative panels in Figure 5; see Appendix B for the full set of surfaces. We take the argument of pericenter ($\omega_2$) and longitude of ascending node ($\Omega_2$) of the perturber to be zero.

As the systems become less hierarchical, physically allowed regions change, particularly for those with an eccentric perturber $e_2 \gtrsim 0.4$. For instance, regions inside $-\pi/2 < \omega < \pi/2$ can be allowed in the mildly hierarchical configurations with an eccentric perturber, as shown in the top right panel in Figure 5. However, the dynamical features typically have a weak dependence on the semimajor axis ratio in the same dynamically allowed regions. Similar to the hierarchical limit, where resonances have been identified at $\omega = \pi/2$ and $3\pi/2$ (Kozai 1962; Lidov 1962) in the quadrupole limit, and at $\omega = \pi$ in the octupole limit in surfaces (Li et al. 2014a), we identify resonances at $\omega = \{\pi/2, \pi, 3\pi/2\}$ in the inner test particle case. Overall, the system becomes more chaotic when it is less hierarchical.

For outer test particle configurations (bottom row of Figure 5), we can see resonances at $\omega = 3\pi/2$ (note that resonances at $\omega = \pi/2$ can also be seen in some surfaces, e.g., middle panel in $e_2 = 0.6, \alpha = 5$ in Appendix B). This is also similar to the hierarchical limit. Specifically, $\omega$ has no resonances at the quadrupole limit, but there are resonances at $\omega = \pi/2$ in the octupole-order Hamiltonian (Naoz et al. 2017). Note that Naoz et al. (2017) identified resonances at $\pi/2$, because they use $\Omega > 0$ as their condition to make the surfaces. To focus on the low-inclination dynamics, we use $\Omega < 0$ instead, since the inclination of points with $\Omega > 0$ are typically over 90°. Similar to the inner test particle cases, as the system become less hierarchical, there are generally more chaotic regions at higher values of $e_2$. The chaotic regions result from overlapping of resonances, and we can see higher-order resonances embedded in chaotic regions (see the panel for $\alpha = 2$, $e_2 = 0.2$).

The colors in the surfaces represent inclination of the particles, which oscillate as the eccentricities vary. For example, trajectories librating around $\omega = \{\pi/2, 3\pi/2\}$ undergo inclination variations that can flip over 90°. Different from the hierarchical limit, orbits can flip from a near-coplanar configuration in a near-circular orbit under the influence of an eccentric outer perturber. We will discuss this in more detail in Section 5.

We now look at surface-of-section plots in $i \cos(\Omega) - i \sin(\Omega)$. We plot the surfaces of sections for systems with the same set of configurations as discussed above. In Figure 6, we show surfaces for $\alpha = \{0.1, 0.3, 0.5, 2, 3, 5\}$ and $e_2 = \{0.6\}$ (see Appendix B for the rest of the surfaces). We chose the surface $\omega = 0$ with the condition $\omega > 0$ to make these plots. Color in this case represents the eccentricities of the test particles. Similar to the surfaces in $e \cos(\omega) - e \sin(\omega)$, physically allowed regions change for mildly hierarchical configurations with highly eccentric outer perturbers. In particular, additional resonant regions show up around $\Omega = 0$ with high inclinations and moderate eccentricities (e.g., top right panel in Figure 6), under perturbations of an eccentric outer object ($e_2 \gtrsim 0.4$) with $\alpha \gtrsim 0.3$.

At low values of $\alpha$, resonances around $\Omega = \pi$ lead to high-eccentricity excitation as the orbits flip cross 90°. In addition, test particle’s orbits circulate when the inclination is close to 0° and 180° due to an eccentric perturber (e.g., top left panel of...
Figure 6). The orbits librate for a wide range of inclinations in between the coplanar and counter-orbiting configurations. To illustrate the flips of the orbit, we marked the circle with a radius of 90°. Many librating orbits cross over 90° at high eccentricities, similar to the hierarchical limit. When the systems become less hierarchical, the eccentricity typically oscillates faster than inclination, and remains low when \( \omega = 0 \). Thus, we find particles with moderate or low eccentricities near 90° on the surfaces (e.g., top right panel of Figure 6). However, the orbits still flip at relatively high eccentricities \( (e > 0.8) \), and the eccentricity when the orbit flips does not show a clear trend as a function of \( \alpha \).

The resonant regions in the plane of \( i \cos \Omega - i \sin \Omega \) are again similar to that in the hierarchical limit. We identify resonances at \( \Omega = \{0, \pi, \pi/2, 3\pi/2\} \) in inner test particle configurations. Note that the resonant regions around \( \pi/2 \) and \( 3\pi/2 \) exist in the surface of, e.g., \( \alpha = 0.3, e_2 = 0.2 \) near \( i \sim 90° \) (as shown in the fifth column in Figure 19 in Appendix B). This is similar to the octupole order, where Li et al. (2014a) find resonances at \( \Omega = \{0, \pi\} \). We can also identify higher-order resonances with high \( (\alpha) \) values embedded in the chaotic sea. Similar to the surfaces in \( e \cos \omega - e \sin \omega \), chaotic regions are more common at higher \( \alpha \) values. For outer test particle configurations, we can identify resonances at \( \Omega = \{\pi/2, \pi, 3\pi/2\} \). This is consistent with the hierarchical limit where, at the quadrupole order, \( \Omega \) is the resonant angle, which librates around \( \Omega = \pi/2 \) (Naoz et al. 2017). Similar to the surfaces shown in \( e \cos \omega - e \sin \omega \), the size of the chaotic regions increases as the systems become less hierarchical.

Different from the octupole level of approximation, the physical regions change when the system becomes less hierarchical. In particular, the region with \( 90° \leq \Omega < 270° \) becomes largely unphysical (e.g., with \( \alpha = \{0.3\}, e_2 = \{0.6, 0.8\} \), and with \( \alpha = \{0.5\}, e_2 = \{0.2, 0.4, 0.6, 0.8\} \)). However, the dynamical features are still analogous to the octupole cases, as mentioned above. In particular, in mildly hierarchical systems (e.g., with \( \alpha = 0.1, e_2 = 0.8 \), with \( \alpha = \{0.3\}, e_2 = \{0.4, 0.6, 0.8\} \), and with \( \alpha = \{0.5\}, e_2 = \{0.2, 0.4, 0.6, 0.8\} \)), libration regions appear near \( i = 90° \) with \( -90° < \Omega < 90° \). The location of these higher-order resonances changes with the value of the energy. At low energies (e.g., in the middle upper panel of Figure 6), these libration regions occur near \( \Omega = \pi/2 \) and \( 3\pi/2 \). As the energy increases, these two libration regions move toward \( \Omega = 0 \). At some point, they overlap and lead to resonances at \( \Omega = 0 \) (e.g., in the upper right panel of Figure 6).

5. Eccentricity and Inclination Excitation

The surface-of-section plots in Section 4 demonstrate that the eccentricity and inclination of the test particles can have large amplitude variations, and this may have important implications for astrophysical systems. In this section, we consider the eccentricity and inclination excitation in detail. First, to illustrate how the eccentricity excitation changes as the system becomes less hierarchical, we show the maximum eccentricity of the test particle as a function of the semimajor axes ratio \( (\alpha) \) in Figure 7 for a circular perturber with a mass ratio \( m_2/m_3 = 3 \times 10^{-4} \). For these simulations, we choose an initial inclination of 60°, greater than the minimum inclination (40°) needed for the Kozai–Lidov mechanism to operate.

Figure 7 shows that, as the semimajor axis ratio increases, so does the maximum eccentricity. While the quadrupole-order expression for the maximum eccentricity \( \epsilon_{\text{max}} = \sqrt{1 - \frac{5}{3} \cos^2 \iota_0} \) is accurate only for \( \alpha < 0.05 \), the semi-analytical results at the eighth order of expansion outlined in Section 3 agree more closely with N-body simulations for higher values of \( \alpha \). For \( \alpha > 0.3 \), this approach also ceases to agree with N-body results and predicts a higher value for maximum eccentricity. This indicates the importance of even higher-order terms of the disturbing function in this regime. The double-average results agree well with the N-body results with the low-mass perturber. With a circular perturber, the maximum eccentricity can be quite large, but it is mostly well below unity.

When the orbit of the perturber becomes eccentric, maximum eccentricity of the test particle becomes more complicated. Previous studies on hierarchical systems at the octupole order showed that the eccentricity of the test particle can be excited to values close to unity, and inclination can be excited to values beyond 90° (Katz et al. 2011; Lithwick & Naoz 2011; Naoz et al. 2011; Li et al. 2014b). Orbits can be flipped (inclination crosses over 90°) in three different scenarios: (1) low initial eccentricity and high initial inclination \( (i > 40° \) and \( i < 140°) \), a scenario similar to the standard Kozai–Lidov mechanism; (2) high initial eccentricity and low inclination; and (3) medium eccentricity and high inclination. When the perturber’s orbit is circular, the dynamics is mainly dominated by quadrupole resonances (as discussed in Section 3), while when the orbit of the perturber is eccentric, both octupole and quadrupole resonances become important (see, e.g., Li et al. 2014a).

We use a numerical approach to study the maximum eccentricity excitation of initially nearly coplanar test particles under the influence of an eccentric perturber. In Figure 8, we show the maximum eccentricity as a function of semimajor axis ratio(\( \alpha \)) for test particles initially aligned (upper panel) and antialigned (lower panel) with respect to an eccentric perturber. The perturber (with \( m_2/m_3 = 3 \times 10^{-4} \)) is on an orbit with an
eccentricity of 0.6, and test particles start on an orbit with $e = 0.4$ and $i = 5^\circ$.

We plot the maximum eccentricity for both inner (left panels) and outer (right panels) test particle configurations. In addition, we consider initially aligned configurations (top panels), where the test particle pericenter starts aligned with that of the perturber, as well as the antialigned configurations (bottom panels). The maximum eccentricity increases as the system becomes less hierarchical for both inner and outer test particles. Except for when the maximum eccentricity is close to 1 or when the test particles are close to mean-motion resonances, double-averaged simulations agree with $N$-body simulations across all values of $\alpha$ shown here. We show maximum eccentricity as calculated using the octupole-level Hamiltonian for inner (Lithwick & Naoz 2011) and outer test particle configurations (Naoz et al. 2017) using green crosses. We can see that the octupole-level Hamiltonian provides a good approximation only for $\alpha < 0.25$ and $\alpha > 2$ in the initially aligned configuration and for $\alpha < 0.1$ and $\alpha > 8$ for the initially antialigned configuration.

It can be seen that when $e_{\text{max}}$ is close to 1, the double-averaged results (blue) are not in agreement with $N$-body simulations (red), due to chaos. To illustrate the effects of chaos, we include results from another double-averaged simulation with initial conditions close to the original simulation (black). We chose the new initial conditions by adding $10^{-4}$ to the original initial conditions in the phase space ($L_1, \omega, J_z, \Omega$). It can be seen that when the system becomes mildly hierarchical ($\alpha \gtrsim 0.18$), the system becomes chaotic, which leads to the discrepancy between the secular and the $N$-body results.

To investigate the eccentricity and inclination variations for different initial eccentricities, we performed an ensemble of secular simulations. We choose the following initial conditions for the test particles: $\alpha \in [0.1, 0.5]$ for inner test particle configurations and $\alpha \in [2, 10]$ for outer test particle configurations, $e_0 \in [0, 0.9]$, $i_0 = 5^\circ$ along with three different initial orientations $\varpi_0 = [0^\circ, 180^\circ, \text{random}]$, where $\varpi$ is longitude of pericenter of the test particle and $e_0$ is the initial eccentricity of the test particle. For the perturber, we choose $e_2 = 0.6$, $\omega_2 = 0$, $\Omega_2 = 0$, and $i_2 = 0$. We evolve the inner test particle systems for a maximum of $10t_p$ and outer test particle systems for $10t_p$ and record the maximum eccentricity and inclination reached in each run. Here, $t_p$ is the Kozai timescale (see Equation (6)), and $t_p$ is the precession timescale given by:

$$t_p = \frac{(m + m_{\text{pert}})^2}{mm_{\text{pert}}} a_{\text{pert}}^2 P,$$

where $m$ is the mass of the central object, $m_{\text{pert}}$ is the mass of the perturber, $a_{\text{pert}}$ is the semimajor axis of the test particle, $a_{\text{pert}}$ is the semimajor axis of the perturber, and $P$ is orbital period of the test particle (Murray & Dermott 2000).

In Figure 9, we show the maximum eccentricity in the plane of the initial eccentricity($e_0$) and semimajor axis ratio$(\alpha)$. The upper panels study the case of an inner test particle. The left panel starts with the aligned configuration, and the middle panel starts with the antialigned one. Similar to the hierarchical limit, starting from a nearly coplanar configuration, it is generally easier to excite the eccentricities as compared to initially aligned ones. In the hierarchical limit at the octupole order, an analytical expression can be derived to predict the flip of an initially nearly coplanar inner orbit (Li et al. 2014b), and we include the criterion using dashed lines in the figures. It shows that the criterion can still be valid up to $\alpha \sim 0.1$ for the antialigned configuration.

The criterion does not predict the flips when the system is initially aligned, because the orbit cannot be flipped starting in the aligned configuration in the hierarchical limit ($\alpha \lesssim 0.1$) at the octupole order (Li et al. 2014b). The right panel corresponds to randomly aligned initial configurations ($\varpi = \text{random}$), and it shows the importance of the initial orientation. Specifically, the eccentricity can remain low for specific values of $\varpi$ even at high values of $\alpha$. This can be attributed to the resonant regions, which can be seen in the surface-of-section plots for high-$\alpha$ configurations.

The lower panel corresponds to the outer test particle configurations. In contrast to the inner test particle cases, starting from a nearly coplanar configuration, the eccentricity is rarely excited close to unity, which would lead the orbits to cross for the outer test particles. This is consistent with earlier results in the literature, which show that up to quadrupole order of the disturbing function, the eccentricity of the outer test particle is constant (Naoz et al. 2017; Vinson & Chiang 2018). Similar to the inner test particles, starting from a nearly coplanar configuration, the eccentricity is more likely to be excited when the orbits are antialigned, and when the system is less hierarchical. Only in antialigned configurations can the secular effects excite to high eccentricities, even in the mildly hierarchical configurations.

It is also apparent that large inclination variations are accompanied by large eccentricity excitations. To illustrate the

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*Figure 8. Maximum eccentricity of initially nearly coplanar test particles as a function of the semimajor axis ratio ($\alpha$) for the inner and the outer test particle configurations with an eccentric perturber. Top panels include particle starting aligned with respect to the perturber, and the bottom panels include those starting antialigned with respect to the perturber. Red dots represent results from $N$-body simulations, blue dots represent secular double-averaged results, and green crosses represent octupole results. To illustrate the effects of chaos, we use gray dots to represent the results from secular double-averaging with a slightly different initial condition ("double avg-2"). Double-averaged results are consistent with $N$-body results across all values of $\alpha$, except when the eccentricity is close to 1, and also at a few points where the particles are trapped in mean motion resonances. Octupole results agree with $N$-body results only when $\alpha < 0.1$ for the antialigned configuration and when $\alpha < 0.25$ for the aligned configuration. For the initially antialigned inner test particle configuration, we also show results from another double-averaged simulation (black) with initial conditions close to the original simulation (blue). These results are not in agreement with the original simulations, which highlights the importance of chaos when the eccentricity is high.*
variations in inclination, we color code the maximum inclination as a function of the initial eccentricity ($e_0$) and semimajor axes ratio ($\alpha$) in Figure 10. The flip criterion in the octupole limit by Li et al. (2014b) is included as black dashed lines, and it is consistent with the double-averaged results for $\alpha < 0.1$ and $\varpi = 180$. At higher values of $\alpha$, the orbits can flip, with lower initial eccentricities as compared to the flip criteria. This is consistent with the results shown in Figure 8. In particular, starting from a near-coplanar configuration, a near-circular inner test particle orbit could flip due to the perturbation of an eccentric outer object starting antialigned with the test particle with $\alpha \sim 0.4$.

For outer test particles (lower panel), starting from a near coplanar configuration, orbit flips are rare unless the orbit starts mildly hierarchical ($\alpha \lesssim 10$) and in an antialigned configuration. This is consistent with Naoz et al. (2017), who find that in hierarchical systems starting from a nearly coplanar configuration, inclination cannot be excited to flip the orbit of the outer particle. Eccentricities are excited close to unity during the flips, and frequently cause the cross of orbits. Similar to the eccentricity excitation, the flips are only seen when the orbits are antialigned.

6. Applications to the Outer Solar System

Mildly hierarchical triples are stable when the perturbing mass is much less massive than the central object, such as in the case of our own Solar System’s extreme trans-Neptunian objects (eTNOs, with large semimajor axes and high eccentricity) under the perturbation of a possible undetected planet residing far from the Sun (Planet 9). In this section, we apply our understanding of the dynamics of the mildly hierarchical triples to the Solar System, and we constrain the properties of the possible undetected Planet 9.

Planet 9 is proposed to explain mysterious features in the orbital distribution of extreme trans-Neptunian object (objects that lie outside the orbit of Neptune with large semimajor axes $\gtrsim 150$ au) (Batygin & Brown 2016; Sheppard & Trujillo 2016). In particular, they show clustering in the longitude of the ascending node, the argument of pericenter, and their orbital planes. Many studies have shown that the alignment of the orbits is not due to selection biases (de La Fuente Marcos & de La Fuente Marcos 2014; Gomes et al. 2015; Batygin & Brown 2016), although Shankman et al. (2017) demonstrated that the “Outer Solar System Origins Survey” (OSSOS; Bannister et al. 2016) contains nonintuitive biases for the detection of TNOs that lead to apparent clustering of orbital angles in their data, and the angular elements of the distant TNOs are consistent with uniform distribution (Bannister et al. 2018). Ongoing observational TNO surveys will provide a better understanding of the architecture of the outer Solar System and the details of the TNO clustering, and it is important to obtain a better understanding of the dynamical origin of possible clusterings of eTNOs.
The proposed Planet 9 is on an eccentric orbit with a large semimajor axis that could perturb the orbits of the eTNOs and explain the clustering of the eTNOs. The underlying dynamics of the interactions between the eTNOs and Planet 9 is rich, and it has been found that secular dynamics plays an important role leading to the clustering of the eTNO orbits (Hadden et al. 2018; Li et al. 2018; Saillenfest & Lari 2017). To illustrate the dominance of the secular resonances, we compare our secular results with those we got from $N$-body simulations below.

In Figure 11, we show the projections for particles orbiting around the Sun at $a = 250 \text{ au}$, under the perturbation of a Planet 9 of mass $m_9 = 10M_\oplus$, with semimajor axis $a_9 = 500 \text{ au}$ and eccentricity of $e_9 = 0.2$. To illustrate the inclination variations and the orbital plane clustering, we show the projections in the plane of $i \sin(\Omega)$ and $i \cos(\Omega)$. The projections are obtained in the same way as the surface-of-section plots in Section 4. We choose the initial condition of the test particle based the results of the surface-of-section plot, so that they start with the same energy. The color represents the eccentricity of the particles. The top left panel shows the results from $N$-body simulations, which do not include the effects of the giant planets. The top right panel, we show $N$-body results that include the effects of the giant planets as a $J_2$ potential. The $J_2$ potential causes precession in $\Omega$, which leads to more frequent orbital crossing. This suppresses the dominance of resonances in $\Omega$ and leads to larger chaotic regions. However, eccentricity excitation near $\Omega \sim 0^\circ$ due to the secular resonances can still be found in the $N$-body results, and this can produce the clustering of the eTNO orbits with high eccentricity. In addition, with the $J_2$ potential, the orbit of Planet Nine is no longer constant. Instead, it undergoes precession, and this causes a slight shift in the resonant region at $\Omega = 180^\circ$.

In the secular results, the orbital elements are obtained relative to the orbit of the outer planet; however, the orbital elements are relative to the ecliptic plane in the $N$-body results. Neptune and other inner planets exert torques that cause Planet 9’s orbit to precess. Thus, to better compare our secular results for mildly hierarchical triples with $N$-body simulations of eTNOs with Planet 9 and the $J_2$ potential, we use mutual coordinates, which are set up as follows. We choose our reference plane and reference direction such that the inclination ($i_9$), argument of pericenter ($\omega_9$), and longitude of ascending node ($\Omega_9$) of Planet 9 are set to 0, following the example of Gronchi (2002).
results based on the mutual coordinates are shown in the bottom left panel, and we can see that the resonance at $\Omega = 0$ is restored in mutual coordinates. The precession due to the $J_2$ potential allows the orbit of the perturber and that of the test particles to cross more frequently. This causes the system to become significantly more chaotic, as shown in Figure 11.

Finally, we include a point-mass Neptune in our N-body simulation (as an active body instead of a $J_2$ term) and show the results in the bottom right panel of Figure 11. Including a point-mass Neptune further suppresses the secular dynamical features. However, we could still see some clustering of the orbit in $\Omega$ with moderate eccentricity at high inclination around $\sim 180^\circ$, due to the secular resonances.

We next ran an ensemble of N-body simulations and constrain the properties of Planet 9. Multiple studies have attempted to constrain the orbital parameters of a potential Planet 9 using N-body simulations. In their original paper, Batygin & Brown (2016) reported that Planet 9 could be a $10M_\oplus$ ($m_9$) planet on an orbit with a semimajor axis ($a_9$) of 700 au, an eccentricity of 0.6 ($e_9$), and an inclination($i_9$) of 30°. These values were updated in a recent paper, where Batygin et al. (2019) find that $m_9 \sim (5, 10) M_\oplus$, $a_9 \sim (400, 800) au$, $e_9 \sim (0.2, 0.5)$, and $i_9 \sim (15-25)^\circ$. The previous studies have focused on configurations of Planet 9 with inclination less that 35°, but it is possible that Planet 9 lies largely out of the plane. Thus, we sample the inclination of Planet 9 over a wide range of inclinations here.

In Table 1, we list the configurations of Planet 9 we use for the N-body simulations. We use 1000 test particles to model the Kuiper Belt. Initial conditions for these particles are listed in Table 2. We also include Neptune as a point particle in our simulations. Other giant planets in the Solar System are modeled using a $J_2$ potential. We use the hybrid symplectic integration method in the MERCURY package to do our simulations. Following Batygin et al. (2019), we use a time step of 10% of the orbital period of the Neptune.

We look for configurations of Planet 9 that would produce the clustering of ETNO orbits. Currently, eight out of nine metastable ETNOs have $\varpi \in [330, 250]$ au and inclination and longitude of ascending node with $\langle \Omega \rangle = \pi$, $\langle \Omega \rangle = 32^\circ$, and $\sigma_{\Omega} = 15^\circ$ (Batygin et al. 2019).

We first calculate the critical semimajor axis $a_c$, beyond which we expect to see clustering. We do this by dividing the simulation data into bins in semimajor axis, and mark the bin where the distribution of $\varpi$ stops being uniform. In our analysis, we look for clustering in the longitude of pericenter by fitting the distribution of $\Delta \varpi = \varpi - \varpi_0$ for $a > a_c$, using the following probability density function:

$$P(x) = (\kappa) \text{uniform}(0, 360) + (1 - \kappa) \text{normal}(x, \mu, \sigma),$$

where $\kappa$ is a measure of the strength of the clustering, where a larger value of $\kappa$ corresponds to less clustering. Here, $\mu$ and $\sigma$ are the mean and the standard deviation of the normal distribution, which denote the location and the strength of the cluster. We calculate the values of $\kappa$, $\mu$, and $\sigma$ for all the simulations we do, and we use the Kolmogorov–Smirnov test to check the goodness of fit. We select the simulations that pass the test in the following analysis.

In Figure 12, we show an example. In the left panel, we plot $\Delta \varpi$ as a function of the semimajor axis ratio for test particles. In this simulation, Planet 9 has a semimajor axis of 700 au with an eccentricity of 0.6, inclination of 0° and mass of 10M_\oplus. We show the critical semimajor axis ratio in black at 260 au for this simulation. The points are sampled from the trajectories of the test particles. Points after two billion years of evolution are chosen at an interval of one million years. On the right, we show the distribution of $\Delta \varpi$ for $a > a_c$ (where $a_c = 260$ au), as well as the fit. For this fit, we find $\mu = 177.7$, $\kappa = 0.321$, and $\sigma = 23^\circ$.

We use association rule analysis to determine which configurations of Planet 9 lead to clustering of the test particles (lower $\kappa$). More specifically, association rule analysis is a machine-learning method used to find relationships between variables in a data set. In the context of this study, each N-body simulation corresponds to a transaction comprised of the orbital parameters of Planet 9 and
The value of the fitting parameter $\kappa$, calculated using the method described above. To use the association rule analysis, we discretize the parameter $\kappa$ as the following:

- $0 < 1 - \kappa < 0.3 \rightarrow \text{low cluster}$
- $0.3 < 1 - \kappa < 0.6 \rightarrow \text{medium cluster}$
- $0.6 < 1 - \kappa < 1 \rightarrow \text{high cluster}$

For example, for the simulation with Planet 9 orbital elements \{a_9 = 300 \text{ au}, e_9 = 0.6, i_9 = 0, m_9 = 5\}, we got $\kappa = 0.55$. This translates to a transaction $t = \{“a_9 = 300\text{au},” “e_9 = 0.6,” “i_9 = 0,” “m_9 = 5,” “medium cluster”\}$.

Association rules are denoted by the notation: $A \rightarrow B$, where $A$ and $B$ are sets of items. Two quantities are used to specify which rules are interesting: support ($s$) and confidence ($c$). Support indicates how frequently a set appears in a data set, and confidence indicates how often the rule is valid. For a given rule $A \rightarrow B$, they are:

$$s = \sigma(A \cup B)/|D|, \quad c = \sigma(A \cup B)/\sigma(A),$$

where $\sigma(A)$ is the count of the set $A$ (i.e., number of times set $A$ appears in the data set) and $|D|$ is the number of transactions in the data set. In this case, $|D|$ is the number of simulations that satisfy the fitting criteria for $\kappa$. Rules with higher support are more widely applicable. Confidence measures the reliability of a rule, and rules with higher confidence are more reliable.

Using rules with $c = 1.0$, we find the parameter space that always leads to orbital clustering. For instance, we find:

$$\{a_9 = 1000 \text{ au}, e_9 = 0.8, i_9 = 90^\circ\} \rightarrow \{\text{high cluster}\},$$

$$\{a_9 = 1000 \text{ au}, e_9 = 0.8, i_9 = 90^\circ\} \rightarrow \{\text{high cluster}\}, \quad (c = 1.0, s = 0.011).$$

This rule tells us that, irrespective of what the mass of Planet 9 is, configurations with $a_9 = 1000$ au, $e_9 = 0.8$, and $i_9 = 90^\circ$ lead to high clustering in $\varpi$.

Other rules with high levels of confidence are listed below:

$$\{a_9 = 700, i_9 = 0, m_9 = 5\} \rightarrow \{\text{high cluster}\},$$

$$\{a_9 = 1400, e_9 = 0.8, i_9 = 90^\circ\} \rightarrow \{\text{high cluster}\},$$

$$\{e_9 = 0.2\} \rightarrow \{\text{low cluster}\},$$

$$\{m_9 = 30\} \rightarrow \{\text{low cluster}\},$$

$$\{c = 0.71, s = 0.16\}.$$

The specific values of the support indicate the size of the parameter space that led to the clustering based on the rules. Thus, rules with fewer Planet 9 parameters (e.g., the third and the fourth rule above) tend to have higher support. While rules with higher support can be applied widely, they tend to have lower confidence, which limits their validity. It should be noted that confidence and support are calculated only for simulations in which $\Delta \varpi$ distribution was a good fit for the test distribution we defined above. Of the 448 simulations we ran, only 276 fit this criteria.

It is intriguing that the high-inclination Planet 9 with a large semimajor axis ($a_9 \sim 1000–1400$ au) on an eccentric orbit ($e_9 \sim 0.6–0.8$) could lead to strong clustering in $\varpi$. This is due to the long secular oscillation timescale of $\varpi$. During the 4 Gyr simulation, $\varpi$ starts to converge to $\sim 170^\circ$ and leads to the clustering.

With high inclinations, the cluster in $\varpi$ may not correspond to clustering in the orbital directions geometrically. To study the geometrical clustering, we find the spread in the pericenter directions directly, following the approach by Millholland & Laughlin (2019). We select particles with pericenter distance between 30 and 100 au and semimajor axis above 250 au for this analysis, since the scattering with the giant planets becomes important when $r_p < 30$ au, and it is challenging to detect the eTNOs with $r_p > 100$ au. Below $a = 250$ au, the clustering is weak due to the fast precession in the $J_2$ potential of the giant planets.

We first estimate the average pericenter direction as the following:

$$\langle \hat{e} \rangle = \frac{\sum_{i=1}^{N} \hat{e}_i}{\sum_{i=1}^{N}},$$

where $\hat{e}_i$ is the eccentricity unit vector of the $i$th test particle, and $N$ is the number of test particles that survived four billion years of evolution residing in the selected parameter region ($30 < r_p < 100$ au, $a > 250$ au). Next, we calculate $\beta_i$, which is the angle between the pericenter orientation of the $i$th test particle and the average pericenter direction. As a measure of the pericenter clustering, we calculate the average values of $\beta_i$ denoted by $\langle \beta \rangle$:

$$\langle \beta \rangle = \frac{\sum_{i=1}^{N} \arccos(\hat{e}_i \cdot \langle \hat{e} \rangle)}{N}.$$
timescales $t_K \lesssim 1 \text{ Gyr}$. In addition, a Planet 9 with a shorter Kozai timescale could also lead to stronger clustering. A retrograde-orbiting Planet 9 with the same dynamical timescale led to the same results as that of the prograde cases. This is because the secular dynamics are independent of the direction of the motion of Planet 9.

When Planet 9 is highly inclined and retrograde ($i_0 \sim 150^\circ$), the massive Planet 9 ($\sim 30 \, M_\oplus$) with a very short dynamical timescale, $t_K \sim 10 \, \text{Myr}$ ($i_0 \sim 300 \, \text{au}$), could also lead to clustering of the pericenters. However, this feature is missing in the prograde scenario, since not enough particles are left in the selected region, as the prograde Planet 9 is more disruptive due to the nonsecular effects. Nevertheless, it is unlikely that Planet 9 lies in this parameter space, because a high-mass Planet 9 with a small and eccentric orbit can mostly be ruled out observationally.

On the lower panel, we plot the average inclination of the selected test particles ($30 < a < 100 \, \text{au}$, $a > 250 \, \text{au}$) versus the inclination of Planet 9. We find that the average inclination can further constrain the inclination of Planet 9. Although both the polar and the planar Planet 9 could produce the clustering, the average inclination produced by the polar Planet 9 is much higher. The current observation of the eTNOs with low average inclination orbits ($\sim 18^\circ$) favors the near-coplanar and the counter-orbiting Planet 9. We note that the observational surveys are not complete for the high-inclination region. The spread of eTNO inclinations due to a polar Planet 9 is large ($\sim 40^\circ$), and selecting only those below $40^\circ$ still shows strong clustering. Thus, current observations cannot yet rule out a polar Planet 9, and future observations of the high-inclination eTNOs are needed to better constrain the inclination of Planet 9.

7. Conclusions

In this paper, we study the secular dynamics of mildly hierarchical triple systems, and apply it to the dynamics of eTNOs in the outer Solar System. In contrast to the hierarchical limit, where one could use a perturbative approach to analyze the dynamics analytically by expanding in the semimajor axes ratio, the dynamics can only be investigated numerically for mildly hierarchical systems. Thus, we developed code to numerically calculate the double-averaged Hamiltonian, and to evolve the system in order to study its secular dynamics. The code is now publicly available (https://github.com/bhareeshg/gda3bd).

In mildly hierarchical systems, the perturbation of a massive object can lead to oscillations that render the secular double-averaged results unreliable. However, the oscillation amplitude is small, and secular results still provide a good approximation when the perturber mass is low. To illustrate this, we calculate the maximum eccentricity induced by the secular interactions and compare that with the $N$-body simulation in Section 3. We obtained an analytical expression for the critical mass, below which the secular results are reliable (Equations (16)) for systems with a circular outer perturber. When the semimajor axes ratio is small $\alpha \sim 0.1$, the critical mass is $m_2/m \sim 0.05$. With higher values of the semimajor axes ratio ($\alpha \sim 0.5$), secular results hold for $m_2/m < 10^{-3.5}$. The critical mass decays with $\alpha^{-3/2}$.

In addition, we make surface-of-section plots to study the dynamics of mildly hierarchical triples and compare these with the hierarchical limit. We find that the secular dynamics have a weak dependence on the semimajor axis ratio $\alpha$ if the perturber does not have a high eccentricity ($e_2 \lesssim 0.8$). For inner test particles, we find secular resonances at $\Omega = \{0, \pi, \pi/2, 3\pi/2\}$ and $\omega = \{\pi, \pi/2, 3\pi/2\}$, and for outer test particles, we find secular resonances at $\Omega = \{\pi, \pi/2, 3\pi/2\}$ and $\omega = \{\pi/2, 3\pi/2\}$. This is similar to the hierarchical limit. The chaotic regions increase as the systems become less hierarchical. In contrast to the hierarchical limit, test particle orbits can flip from a near-coplanar configuration starting with low eccentricities.

We then study the eccentricity and the inclination excitation of the test particles inside the mildly hierarchical triples. For circular perturbers, we obtain semi-analytical results for the maximum eccentricity with an eighth-order expansion in the semimajor axes ratio, which agrees with the $N$-body results up to a semimajor axes ratio of $\alpha \sim 0.3$ (Section 3). For an eccentric perturber, double-averaged results and $N$-body results agree well with each other, while octupole results typically give higher $e_{\text{max}}$, when $\alpha \gtrsim 0.1$. We then perform an ensemble of secular simulations, and find that the eccentricity is easily
excited for initially antialigned systems and for less hierarchical systems.

Finally, we apply our results to objects in the outer Solar System. The secular dynamical features resemble that of the $N$-body results for the eTNOs under the perturbation of the undetected outer planet (Planet 9). Using surface-of-section plots, we find that the secular resonances can lead to clustering in eTNO orbits. Next, we perform an ensemble of $N$-body simulations to model the interactions between Planet 9 and eTNOs. In addition to a low-inclination Planet 9 as identified in the literature (e.g., Batygin et al. 2019), we find that a polar ($i_9 \sim 90^\circ$) and a counter-orbiting ($i_9 \sim 180^\circ$) Planet 9 with Kozai timescales of $\lesssim 1$ Gyr (for an eTNO with $a = 250$) could also produce strong clustering. A high-inclination or a counter-orbiting Planet 9 could pose challenges to the formation of such a highly inclined wide-orbit planet, which may indicate that Planet 9 could be a captured planet from another star (Li & Adams 2016). The near-coplanar and the counter-orbiting Planet 9 could lead to low-inclination eTNOs (average inclination of $\sim 20^\circ$), while the polar one leads to higher-inclination $\sim 60^\circ$ eTNOs with a large spread $\sigma_i \sim 40^\circ$. Future observations of the eTNOs with high inclinations could better constrain the Planet 9 inclination.

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### Appendix A

**Numerical Accuracy and Integration Methods**

To ensure consistency in our $N$-body results, here we compare various integration schemes and choices of time steps. In the left panel of Figure 14, we show the maximum eccentricity (reached in $3t_K$) as calculated using the double-averaged simulation (da) and $N$-body simulations. Two different integration methods were used for $N$-body simulations (with Mercury simulation package): Bulirsch–Stoer algorithm (bs) and hybrid methods. Each of these methods were run with three different time steps: 2.5%, 5.0%, and 10% of the period of the innermost orbit. In the right panel, we show the relative difference in maximum eccentricity with respect to the maximum eccentricity computed by the different algorithms with the different time steps.

The hybrid integration scheme with different time steps does not agree well when the eccentricity is high. Hence, we chose to use the Bulirsch–Stoer integration scheme for our $N$-body simulations. The Bulirsch–Stoer method agrees very well with the secular double-averaged simulations for all three of the time steps that we chose, except when the configuration is near mean-motion resonances, which are highlighted using dashed black lines. When alpha becomes larger than $\sim 0.18$, the system becomes chaotic (e.g., Figure 8), so results at different time steps with different integration methods no longer agree with each other. Numerical accuracy is high enough not to affect the maximum eccentricity.

![Figure 14](image_url)

**Figure 14.** Comparison of various integration schemes and time steps. Left panel: We plot the maximum eccentricity as a function of semimajor axis ratio for different integration schemes and time steps. We show results for Bulirsch–Stoer integrator (bs) and hybrid integrator (hybrid) with time steps of 2.5%, 5.0%, and 10% of the period of the innermost orbit. Right panel: We show the relative difference in maximum eccentricity. Hybrid integration scheme does not agree very well at high eccentricity. Also, double-averaged results (da) agree with $N$-body results when the system is not near mean-motion resonances (black dashed lines). Initial conditions are same as those used in Figure 8.
Appendix B
Additional Surface-of-section Plots

In this section, we present all the surface-of-section plots for different semimajor axis ratios $\alpha = \{0.1, 0.2, 0.3, 0.5, 2, 3, 5\}$ and perturbers eccentricities $e_2 = \{0.2, 0.4, 0.6, 0.8\}$. In Figures 15–22, each row corresponds to a different $\alpha$, and each figure corresponds to a different outer binary eccentricity $e_2$.

For a given configuration of the system, only a finite range of Hamiltonians are physically allowed. To select the energy levels used to make the surfaces in $e - \omega$ space, we sample the values of $H$ on a grid in $e \cos(\omega) - e \sin(\omega)$ with $\Omega = 0$. We then collect the $H$ values at the grid points, and choose the mean ($\langle H_{\text{grids}} \rangle$) as well as one and two standard deviations away from the mean ($\langle H_{\text{grids}} \rangle \pm \sigma_{H_{\text{grids}}}$ and $\langle H_{\text{grids}} \rangle \pm 2\sigma_{H_{\text{grids}}}$) to be the energy levels in the surfaces. The different columns in Figures 15–22 correspond to the different energy levels. We follow a similar procedure to select energy levels for surfaces in $i - \Omega$ space.

By looking at different surface-of-section plots in a given row (with the same semimajor axes ratio), it is clear that the dynamics depends sensitively on the value of the Hamiltonian. Eccentricities are generally excited to higher values when the energy is low for inner test particles, while it is the opposite when the test particle is in the outer orbit. Various features of these surfaces are presented in detail in Section 4.

Figure 15. Surface of section in $e \cos(\omega) - e \sin(\omega)$ space for $e_2 = 0.2$. To choose our points, we use the conditions $\Omega = 0$ and $\dot{\Omega} < 0$ for inner test particle configurations and $\Omega = \pi/2$ and $\dot{\Omega} < 0$ for outer test particle configurations.
Figure 16. Same as Figure 19, except for $e_4 = 0.2$. 

$e_2 = 0.4$
Figure 17. Same as Figure 19, except for $e_2 = 0.6$. 
Figure 18. Same as Figure 19, except for $e_2 = 0.8$. 
Figure 19. Surface of section in $i \cos(\Omega) - i \sin(\Omega)$ space for $e_2 = 0.2$. We use the conditions $\omega = 0$ and $\dot{\omega} > 0$ to choose our points.
Figure 20. Same as Figure 15, except for $e_2 = 0.4$. 
Figure 21. Same as Figure 15, except for $e_2 = 0.6$. 
**Figure 22.** Same as Figure 15, except for $e_2 = 0.8$.  

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