Origin of Earth's Water

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N-body simulations of primordial Solar Systems are used to investigate possible sources of Earth's water. It is found that Jupiter's gravitational influence can perturb water-rich planetary embryos from the outer asteroid belt to the inner Solar System where they can collide with dry embryos. A net motion of water from 3.4 ± 0.1 AU to 3.0 ± 0.3 AU is measured. This is a major source of water delivery in the early Solar System and is likely the primary source of Earth's water. It is found that primordial Jupiter-family comets are cleared rapidly within 10^4 yrs and that collisions between comets and Earth account for less than 20% of Earth's water.

I Introduction

The 'Goldilocks Zone' is the region around a star in which an orbiting planet could support liquid water on its surface; arguably the most important factor in determining whether it can harbour life. However, there exists a troubling paradox in this definition. The star's heat and stellar wind mean that water can only exist as steam in the inner system and only as ice in the cold outer system. All material in the inner system will therefore be much drier than material in the outer system (the boundary between these wet and dry areas is known as the frost line). This is evidenced by the water content of asteroids in the Solar System which varies from 0.1-10% between the inner and outer asteroid belt [1]. Any planet with a temperature high enough to support liquid water must be within the frost line, and since planets are formed via the accretion of asteroids in their immediate neighbourhood, we have a paradox: that wet planets are made from totally dry constituents. The origin of water on wet, habitable planets such as Earth is an actively debated topic and has vast implications about our understanding of terrestrial planet formation and the abundance of life in the universe.

During the first $\sim$10Myr of the Solar System's life, innumerous small grains of material ($\sim$1cm diameter) accumulated via accretion to eventually form larger planetesimals ($\sim$1km diameter). At this critical size, larger planetesimals began to accrete material at a greater rate (oligarchical accretion) leaving 20-50 planetary embryos ($\sim$1000km diameter) dominating the inner solar system which will eventually collide to become planets over the next $\sim$ 100Myr [2]. Before these giant collisions, the embryos within the frost line were dry. The origin of Earth's water is believed to be due to a process that takes place after this point.

One possible mechanism for water delivery to the inner Solar System is the depletion scenario. It is known that the asteroid belt was once $10^2 - 10^3$ times as massive as it is today [3] and that Jupiter's gravitational influence is the primary cause of this depletion [4]. Jupiter is the oldest planet and a proto-Jupiter likely existed during the epoch of embryo formation [5]. Primordial bodies that encountered Jupiter would have either been ejected on hyperbolic orbits or have spiraled inwards. Since Jupiter's influence is greater outside the frost line than within, we expect wet bodies to be perturbed inwards disproportionately more often than dry bodies being pulled outwards. Collisions between the dry embryos and perturbed wet bodies are now possible, this would hydrate them and explain the paradox. Simulations suggest that the speed of embryo formation is inversely proportional to orbital radius [6] so it is reasonable that the inner solar system is populated with embryos while the asteroid belt is populated with planetesimals. This is the leading mechanism and it has been shown to produce realistic systems with Earth-like planets in simulations[7]. Depending on exactly when Jupiter formed, this mechanism may also have taken place later, when the outer asteroid belt contains water rich embryos which also get perturbed into the inner Solar System. It can be shown that this mixture of planetesimals and embryos in the asteroid belt produces reasonable planets and that a small number of embryo-embryo collisions can deliver similar quantities of water to many thousands of embryo-planetesimal accretions [8]. This report will investigate the possibility that the depletion scenario happened at an even later stage of Solar system evolution, where planetary embryos have formed all the way up to the outer asteroid belt (emptying it of planetesimals), and explore whether a realistic planetary system can develop in a reasonable timescale.

The simulation results for the depletion scenario are supported by geochemical analyses of primordial asteroids. Carbonaceous chondrites are an ancient, water-rich ($\sim 10\%$ water) species of asteroid abundant in the early solar system. The bulk hydrogen and nitrogen isotopic compositions of chondrites are very similar to Earth's, suggesting that they are the principal source of these elements [9]. In particular, the mean deuterium/hydrogen (D/H) ratio of chondrites is $(140 \pm 10) \times 10^{-6}$ which is in excellent agreement with Earth's $(149 \pm 3) \times 10^{-6}$ [10]. It follows that, if the depletion scenario is correct, embryos from beyond the frost line that spiral into the Goldilocks zone and collide with a proto-Earth are likely comprised of chondritic material.

After giant collisions between embryos form planets, the inner Solar System remains stable for billions of years. If the depletion scenario delivered insufficient water to the embryos that would become Earth, there must be an alternative delivery mechanism that: 1) happens much later in the Solar System's life and 2) sources water from outside the now stable terrestrial bodies. The late veneer scenario is one such mechanism which posits that Earth received a bombardment of comets after the main stage of planetary formation, a so-called 'late veneer'. Comets contain large amounts of ice so relatively few collisions are needed to provide an embryo with sufficient water. This report will explore the extent to which Jupiter-family comets are responsible for delivering Earth's water by investigating their behaviour in an analogue of today's Solar System.

The current consensus is that the late veneer is a minor contributor to Earth's water ($< 10\%$ for Kuiper belt comets and $2 - 20\%$ for Jupiter-family comets). This has been calculated analytically [1] and is backed up experimentally by comparisons between the D/H ratios of comet ice and Earth's oceans. Earth's bulk D/H ratio is much lower than those of comets (Halley's comet has a value $(310 \pm 30) \times 10^{-6}$ for example). However, since only a handful of comets have had their D/H ratio measured, this result is not conclusive.

This report will use N-body simulations to model water delivery mechanisms to Earth. First the computational methods and algorithms will be discussed, then methods and results for each scenario will be presented separately. These will be summarised and placed within the context of current literature followed by topics of further investigation.

II Computational Methods

Planetary systems are modelled as a system of N gravitationally interacting, rigid particles whose positions are evolved using the leapfrog algorithm. The force on one particle i is given by summing over the Newtonian gravitational force between i and all other particles j:

$$\boldsymbol{F}^i = G \sum_{j \neq i} \frac{-m^i m^j}{|\boldsymbol{r}_{j \to i}|^2} \hat{\boldsymbol{r}}_{j \to i} \tag{1}$$

Using Newton's second law, this can be trivially integrated to give the equations of motion for all particles in the system. However, over many time steps, numerical inaccuracies can occur if these are used unaltered. In particular, calculating the position and velocity together at integer time steps has an error of first order $\sim dt$ (where dt is the time difference between steps or simply 'time step'). This is reduced to second order $\sim dt^2$ by staggering the position and velocity calculations half-steps apart (where $n \in \mathbb{Z}$ is the step number):

$$\boldsymbol{v}^i_{n+1/2} = \boldsymbol{v}^i_{n-1/2} + \frac{\boldsymbol{F}^i_n}{m^i} dt \tag{2}$$

$$\boldsymbol{r}^i_{n+1} = \boldsymbol{r}^i_n + \boldsymbol{v}^i_{n+1/2}\, dt \tag{3}$$

Here, force is calculated from position at step n and used to evolve velocity between $n - 1/2$ and $n + 1/2$. Velocity at $n + 1/2$ is then used to evolve position from n to $n + 1$. This way, position and velocity get calculated in an alternating pattern and are said to 'leapfrog' over eachother. Although more accurate algorithms exist (e.g. Runge-Kutte with error $\sim dt^4$), the leapfrog algorithm was chosen since it is simple, computationally efficient and is time reversible. Crucially, it approximately conserves the energy of the system as long as time step is low enough. However, energy must be calculated using position and velocity at the same step. The Verlet velocity can be added to the leapfrog algorithm to evolve velocity at half-steps to achieve this:

$$\boldsymbol{v}^i_n = \boldsymbol{v}^i_{n-1} + \frac{1}{2} \frac{\boldsymbol{F}^i_n}{m^i} dt \tag{4}$$

Time step must be chosen carefully. A small step is desirable since it evolves the system with a smaller error and means the simulation's values numerically converge towards the true values. However, small time steps mean that the simulation is computationally expensive and will take a long time to evolve the system over many 'years' for the N bodies. The reverse is true for a large time step: many simulated years will pass very quickly but the results may not numerically converge. By testing the code on a simple Solar System of Earth, Jupiter and the Sun, it was found that a time step of $dt = 5$ days was appropriate.

Two Bodies passing nearby is a problem for simulations with time steps much larger than the time taken for them to pass each other. During their close encounter, the bodies exert large forces on each other. If the time step is large then the resolution of the system is insufficient to properly evolve the bodies' orbits and can result in bodies being unrealistically ejected by the huge forces. To solve this, a softening factor ϵ can be added to equation 1 such that the force is greatly decreased during close encounters but is changed negligably at large distance:

$$\boldsymbol{F}^i = G \sum_{j \neq i} -m^i m^j \frac{\boldsymbol{r}_{j \to i}}{(|\boldsymbol{r}_{j \to i}|^2 + \epsilon^2)^{3/2}} \tag{5}$$

However, this is computationally more expensive than equation 1. Fortunately, since the code is simulating collisions, the bodies will collide before the forces become unrealistic. This is achieved by merging bodies that are within some threshold distance of eachother. This threshold is proportional to a body's radius multiplied by some scaling factor s. This must also be chosen carefully since if it is too great then collisions will happen unnecessarily; but if it is too small then unreal forces may still be present. Preliminary simulations of colliding test particles found $s = 100$ to be appropriate. Collisions were modelled as perfectly inelastic and with no fragmentation. The two bodies coalesce into a new body with a new velocity that obeys conservation of momentum. Clearly, a real collision between embryos would be much more complex than this, however modelling this would require each body to be made of many smaller particles and be computationally expensive.

III Depletion Scenario

A. Methods

Each simulation begins from a system in the latter stages of planetary development, where planetary embryos have formed throughout the inner Solar System and emptied the asteroid belt of planetesimals. Twenty planetary embryos were placed between $0.5 - 4.5$ AU in the ecliptic such that their orbital radii were equidistant from each other but at a random angle around the Sun. This ensures that the embryos are equally distributed radially away from the sun but that there is no pattern or systematic error in their initial positions. Each embryo had a mass of 5.9×10^{23} kg such that their collective total mass was equal to the total mass of the terrestrial planets today 1.18×10^{25} kg [11]. Embryos are thought to have masses between the lunar and martian mass [7]. The embryos in these simulations are within the upper end of this range, being slightly lighter than Mars.

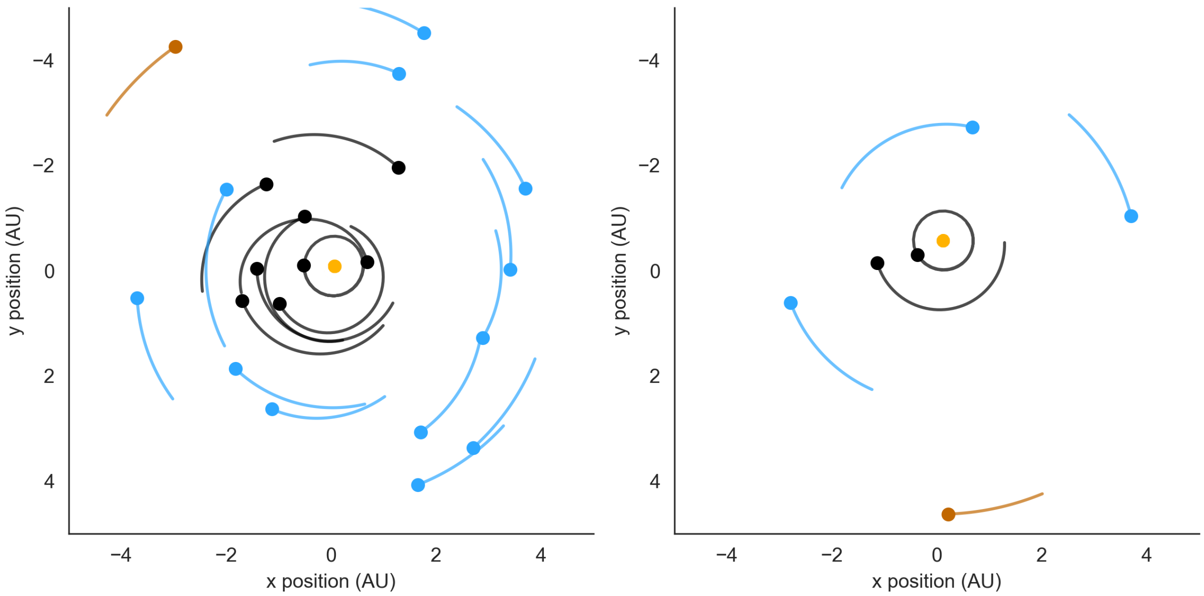

FIG. 1: The initial (left) and final (right) states of one of the depletion simulations. Embryos containing water are shown in blue and dry embryos are black, the Sun and Jupiter are shown in yellow and brown respectively. Initially, there are many embryos and the wet embryos orbit far from the sun. After giant collisions, a realistic Solar System is formed with few larger planets, some of which are hydrated. Bodies have 250-day long trails.

The embryos are yet to settle into stable orbits. To model this, each embryo was perturbed slightly from a perfect circular orbit. A random number δ_x was chosen from a gaussian distribution with a mean of 1 and standard deviation of σ and multiplied with the x component of the perfect circular velocity c to get the embryo velocity in the x direction (and similarly for y):

$$\begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} \delta_x c_x \\ \delta_y c_y \end{pmatrix} \;\forall\, \delta \sim N(1, \sigma^2) \tag{6}$$

Different random numbers were calculated for x and y to ensure there was no correlation between them and that the final velocity vector was truly random. It was found that $\sigma = 0.1$ was appropriate for producing a reasonable distribution of embryo orbits that were not unrealistically eccentric or circular.

The embryos all had a density equal to the mean density of carbonaceous chondrites: 3440 kgm^{-3} [12]. The frost line was taken to be 2 AU. Embryos within the frost line are totally dry. Embryos between 2-4.5 AU are wet and have a random water percentage following a gaussian distribution of $(10 \pm 3)\%$, consistent with chondrites. Similarly, wet embryos had a randomly selected D/H ratio, chosen from a gaussian distribution following the D/H ratio of chondrites: $(140 \pm 10) \times 10^{-6}$.

Each simulation used a different seed so that the computationally generated random numbers were distinct between simulations. Ten individual simulations were conducted and their results combined to explore their general behaviour. Each simulation ran for one million time steps.

B. Results & Discussion

All ten of the simulations evolved the system of twenty embryos into a realistic system of fewer planets. A typical example is shown in figure 1. The greatest number of planets formed in a given simulation was ten and the smallest was four, on average the simulation ended with a reasonable 6.9 ± 0.5 planets. Although this is much greater than our Solar System, it has been observed in exoplanet systems such as the TRAPPIST-1 system with 7 rocky planets [13].

Since rocky exoplanets are so difficult to detect, their initial mass function is unknown. It is therefore difficult to place these simulation results in a wider context beyond our Solar System. The average mass of all the bodies after the simulation was $(1.4 \pm 0.1) \times 10^{24}$ kg. This is in reasonable agreement with the mean mass of real terrestrial planets of $(3 \pm 1) \times 10^{24}$ kg. It appears though that the simulation consistently produces medium size planets around 3 Mars Masses and rarely produces larger Earth or Venus size planets. This is due to leftover embryos that haven't yet had time to collide to form a planet. By ignoring these, we find the average mass of planets formed from at least two embryos was $(2.3 \pm 0.3) \times 10^{24}$ kg. The simulations created two Earth-like planets (defined as as a weighing above 4×10^{24} kg and orbiting within 2 AU) with masses 4.13×10^{24} kg and 5.31×10^{24} kg, very similar to Venus which has mass 4.87×10^{24} kg. We have that 20% of simulations produced an Earth-like planet and 100% of simulations produced planets made from multiple embryos. 20.3% of all planets were made from more than 1 embryo and 3% were Earth-like.

The simulations clearly demonstrated the transfer of water from beyond the frost line to the inner Solar System. This is shown in figure 2. The final planets have much lower semi-major axes than the initial embryos, showing a clear motion of wet bodies towards the inner system as the action of Jupiter depletes the asteroid belt area. By taking the average semi-major axis of the bodies and weighting them by water content, we can find the average position of water in the system. Across all ten simulations, the average water position moved inwards from 3.4 ± 0.1 AU to 3.0 ± 0.3 AU.

The exact amount of water within Earth's mantle is poorly constrained, but it is thought that some several oceans of water are sequestered [14]. Taking one ocean to be $\sim 10^{21}$ kg, Earth may contain up to $\sim 10^{22}$ kg of water, giving it a water mass fraction of ~ 0.01. The simulated Earth-like planets have water mass fractions of 0.07 and 0.06 respectively. It is reasonable that these are overestimates, since it was assumed that no material was lost during collisions and all of the wet embryos were water-rich carbonaceous chondrites. Hence the water content of Earth and the simulated Earth-like planets are comparable. It is estimated that The D/H ratios of the Earth-like planets are 145×10^{-6} and 139×10^{-6}, in good agreement with Earth's. Therefore the depletion scenario is a major source of Earth's water. It is worth noting that, although embryos were only placed up to an orbital radius of 4.5 AU, the initial perturbations in their velocity can change their semi-major axis to values greater than this. This is why a minority of initial embryos are beyond 4.5 AU in figure 2.

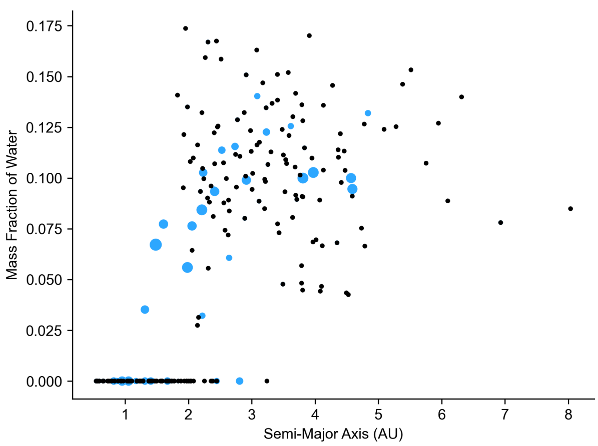

FIG. 2: Water content of planets as a function of their Semi-Major Axis across all ten simulations. The initial distribution of embryos are shown in black and the formed planets are shown in blue. The sizes of the points are relative to the body's mass.

Slightly eccentric embryos are more likely to cross orbits with other embryos and collide to form a planet. Therefore we expect the mean eccentricity to decrease during planet formation. Initially the mean eccentricity is 0.143 ± 0.007 and becomes 0.126 ± 0.009 after planet formation. This is a decrease of $2.43\ \alpha$, only a slight decrease. This is in good agreement with the mean eccentricity of real planets of 0.08 ± 0.04. However these simulations appear to produce Earth-like planets that are too eccentric. Earth and Venus have eccentricities of 0.017 and 0.007 respectively, whereas the Earth-like simulated planets have values of 0.179 and 0.235.

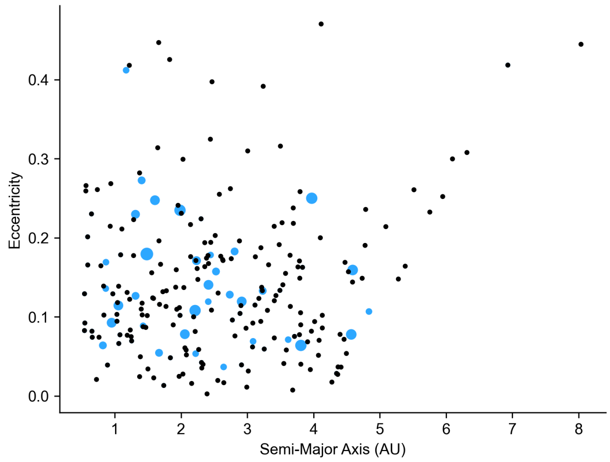

FIG. 3: Eccentricity of planets as a function of their Semi-Major Axis across all ten simulations. The initial distribution of embryos are shown in black and the formed planets are shown in blue. The sizes of the points are relative to the body's mass.

The simulations ran for one million steps since preliminary experiments running up to ten million showed that planetary formation had largely finished by this point. The large mean eccentricity and occasional leftover embryos suggests that further formation may occur at a later date. With greater computational power, the code could be run for one hundred million steps to check if this is the case. With a time step of 5 days, one million steps is approximately 10^4 yr. Modelling the depletion scenario at an earlier stage, with embryos within the frost line and planetesimals in the asteroid belt, predicts that this process takes $\sim 10^8$ yr. The presented simulations have found that the lifetimes of embryos in the asteroid belt are very short and get scattered by Jupiter in $\sim 10^4$ yr. Hence, if Jupiter moved into its current orbit late in Solar System evolution, or an embryo got ejected to the asteroid belt, planetary formation will still happen as normal and manage to produce life-supporting, wet planets.

IV Late Veneer Scenario

A. Methods

Each of the ten simulations begin in a simplified, old Solar System in which stable planets have been formed. The system contains the major terrestrial planets Earth, Venus and Mars; and the gas giants Jupiter and Saturn placed in circular orbits around the Sun. One hundred comets are placed in the Jupiter-Saturn region between 4.5-10 AU and are given orbits using the same method as described in section III A. Since comets are more eccentric than planetary embryos, here σ was set to 0.5 to ensure a wider range of initial velocities and hence a higher eccentricity. Jupiter-family comets have a low-inclination so a 2D simulation is appropriate, unlike comets from the Kuiper belt and Oort Cloud. The motion of Jupiter-family comets is dominated by Jupiter and Saturn so the ice giants Uranus and Neptune have been omitted for computational speed. The masses of the comets are negligible compared to the planets, so they have been evolved as test particles to improve the efficiency of the program. For purposes of water delivery: the comets have typical comet masses of 10^{13} kg and are 100% water.

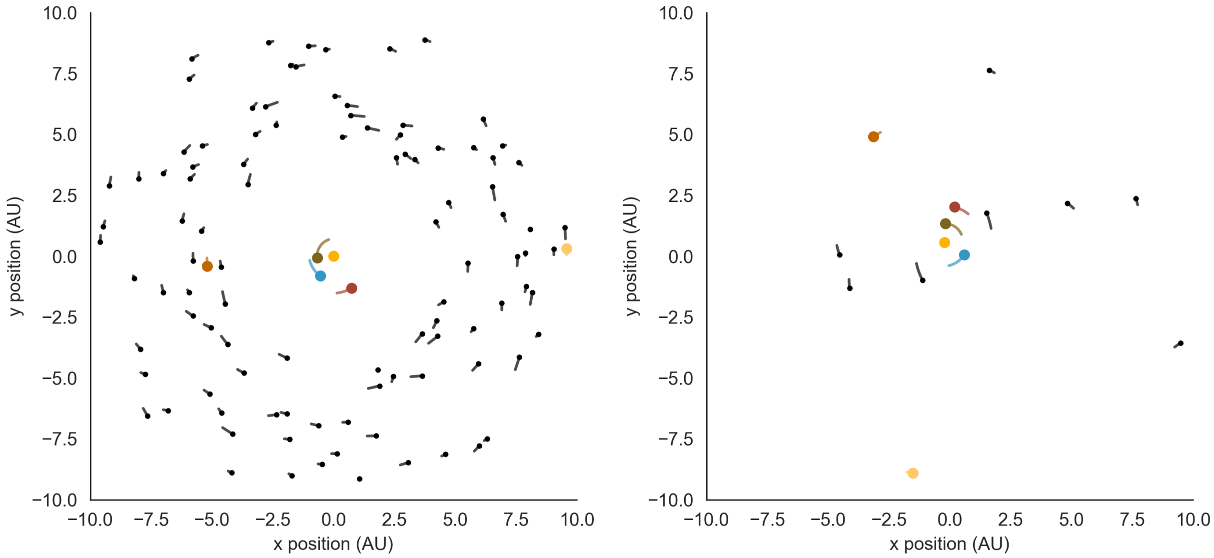

FIG. 4: The initial state (left) and final state (right) of one of the late veneer simulations. The Sun, Venus, Earth, Mars, Jupiter and Saturn are shown as large, coloured points and the comets are small black points. Each body has a 50-day trail.

They have D/H ratios randomly selected from a normal distribution of $(310 \pm 30) \times 10^{-6}$. This is the D/H ratio of Halley's comet and is typical of the few comets that have been measured [10].

B. Results & Discussion

In 10^4 yr, 92% of comets have been cleared from the Jupiter-Saturn region. This is in agreement with literature which finds that the region is cleared by 10^5 yr [1]. This is shown in figure 4. Only 0.02% of comets collided with Earth. Each simulation modelled one hundred comets, meaning there was 10^{14} kg of water held in comets per simulation. It is estimated that in reality there was $\sim 10^{25}$ kg held in comets at this time. Therefore simulations suggest that $\sim 2 \times 10^{21}$ kg of cometary material should have been delivered to Earth, this is roughly equivalent to 1.3 oceans worth of water if the comets are 100% ice and all of their material is perfectly absorbed. Given that several oceans of water are believed to reside in the mantle [15], this is in reasonable agreement with estimates that comets only account for 2-20% of Earth's water [1].

V Conclusions & Extensions

This report has presented N-body simulations that investigated two different scenarios which could explain the apparent paradox in the origin of Earth's water. When investigating the depletion scenario, the simulation generated realistic systems from sets of twenty planetary embryos. These systems matched today's Solar system in: mean mass and water content, mass and D/H ratio of Earth-like planets. This agrees with the literature consensus that the primary source of Earth's water was via accretion of water rich bodies from beyond the frost line. It is found that the lifetime of embryos beyond the frost line is very short relative to the planetary formation time. The simulation failed to replicate the eccentricity or timescale of real systems. In future, this work could be extended by running the code over a greater number of steps on a more powerful computer to determine whether the planets settle into more circular orbits over time.

To investigate the late veneer scenario, the simulation evolved one hundred Jupiter-family comets in an analogue of today's Solar System. It was found that less than 20% of Earth's water likely came from comets, agreeing with literature that it is likely a minor source of Earth's water. A more powerful computer could run this code for more steps and with more comets or perhaps investigate the contribution of comets from other regions of the Solar System.

Recently, a third scenario for water delivery was proposed [15] where Earth absorbs 1% of its water from the Solar Nebula as hydrogen. No simulation is yet to include this nebular ingassing. Future simulations could aim to include all three scenarios together and generate a realistic Solar system from the very beginning of planetary formation, as opposed to simulating each scenario separately as presented here.

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