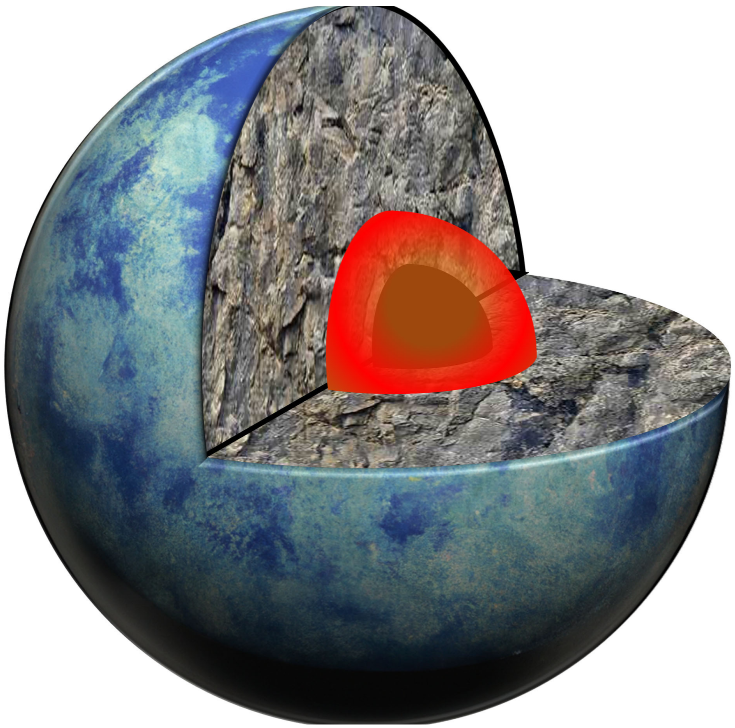
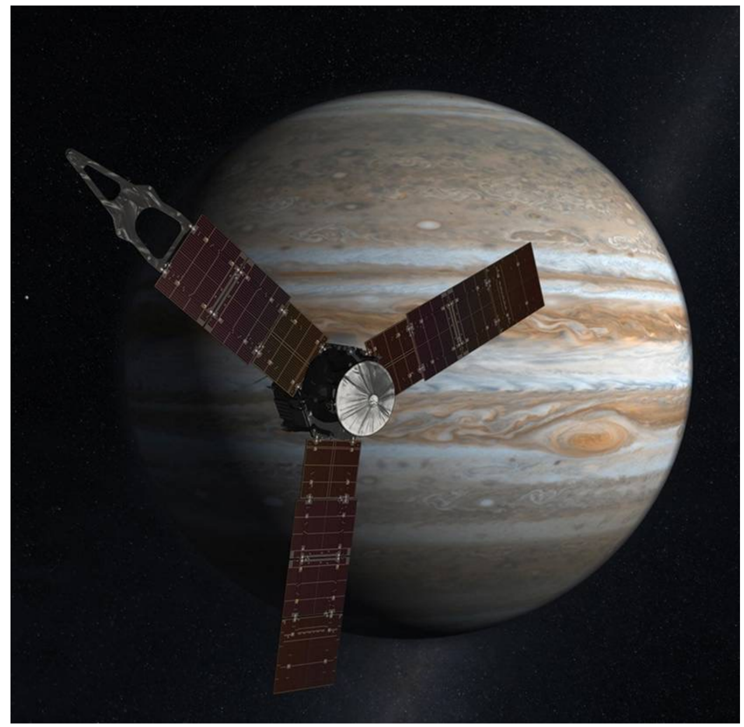
Ab initio Simulations of Iron
NASA mission Juno to Jupiter & dilute core





Burkhard Militzer

UC Berkeley

Ab initio Simulations of Iron
NASA mission Juno to Jupiter & dilute core

L5: Path integral Monte Carlo (PIMC) simulations and First Principles Equation of state (FPEOS) database

L9: EOS of iron, NASA mission Juno to Jupiter

T1: "Build that Planet" with SPH method

L12: NASA mission Cassini to Saturn. How did that planet become the Lord of the Rings?

T3: FPEOS tutorial

Big Questions that my Group Helps Address

1. How did our solar system form?
2. What are giant planets made of?
3. How do material behave at high pressure?

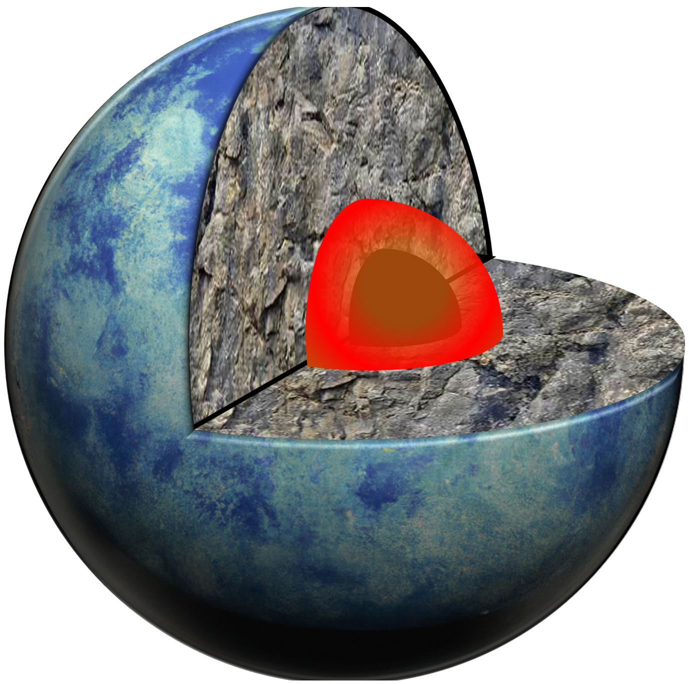
Outline

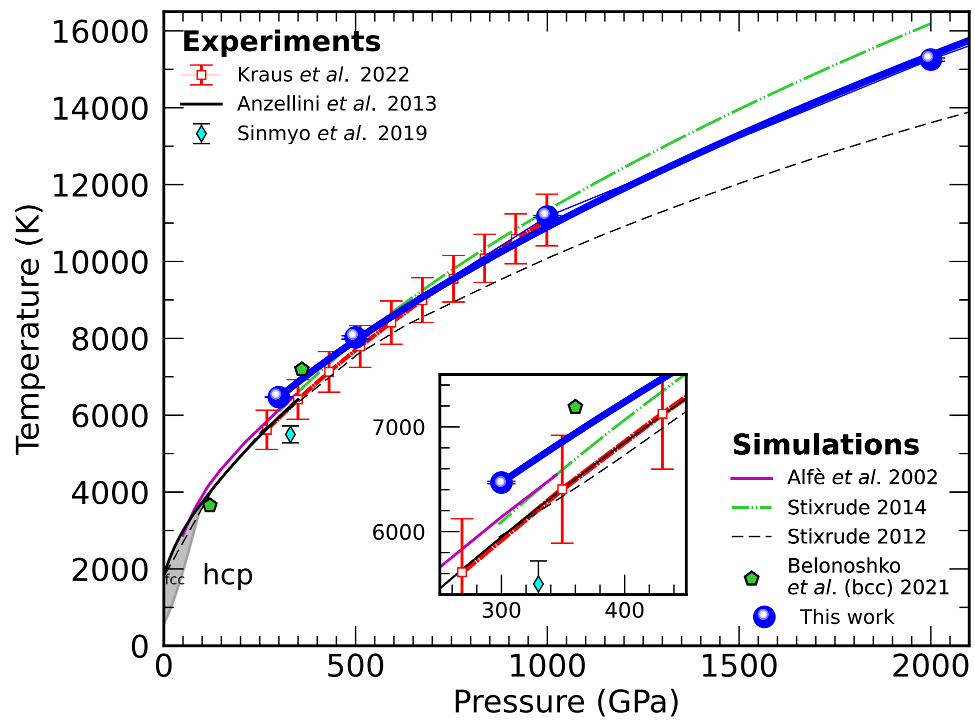
1. Equation of State and Melting Line of **Iron** at Megabar pressures
2. Juno mission and **Jupiter's Dilute Core**
3. **Quadratic Monte Carlo** – a general-purpose sampling method

1. Iron Melting

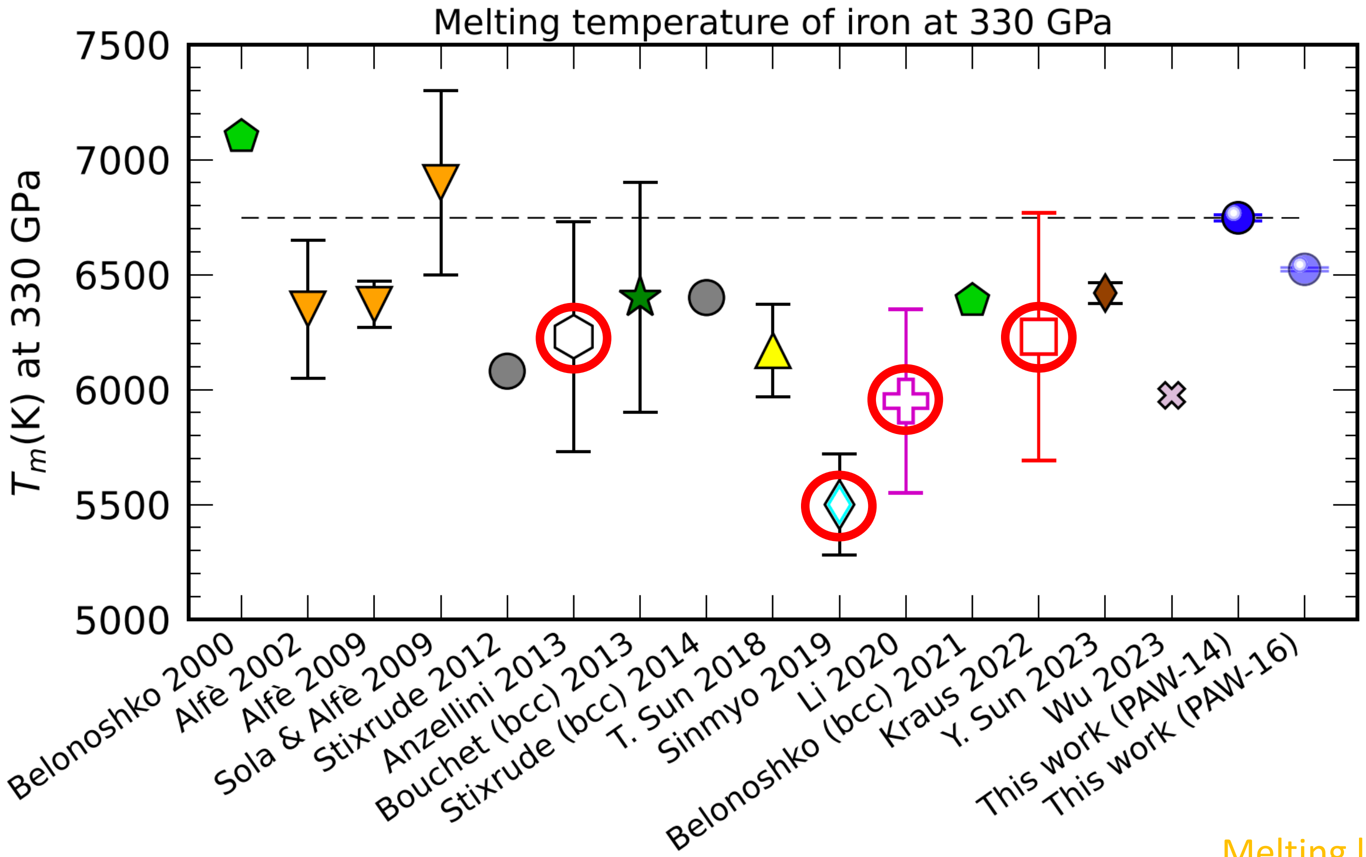
Iron melting at terapascal pressures and core crystallization of Super-Earths Planets

F. Gonzalez-Cataldo, B. Militzer, "Ab initio determination of iron melting at terapascal pressures and Super-Earths core crystallization", Physical Review Research 5 (2023) 033194



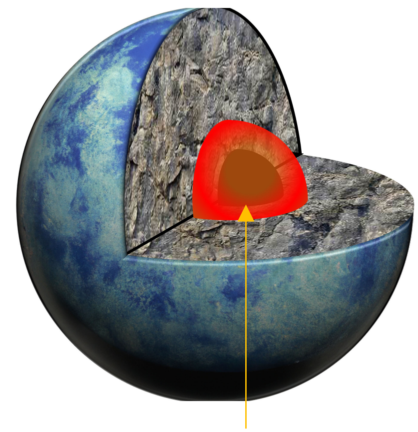


Melt temperature at 330 GPa, Earth's inner core boundary



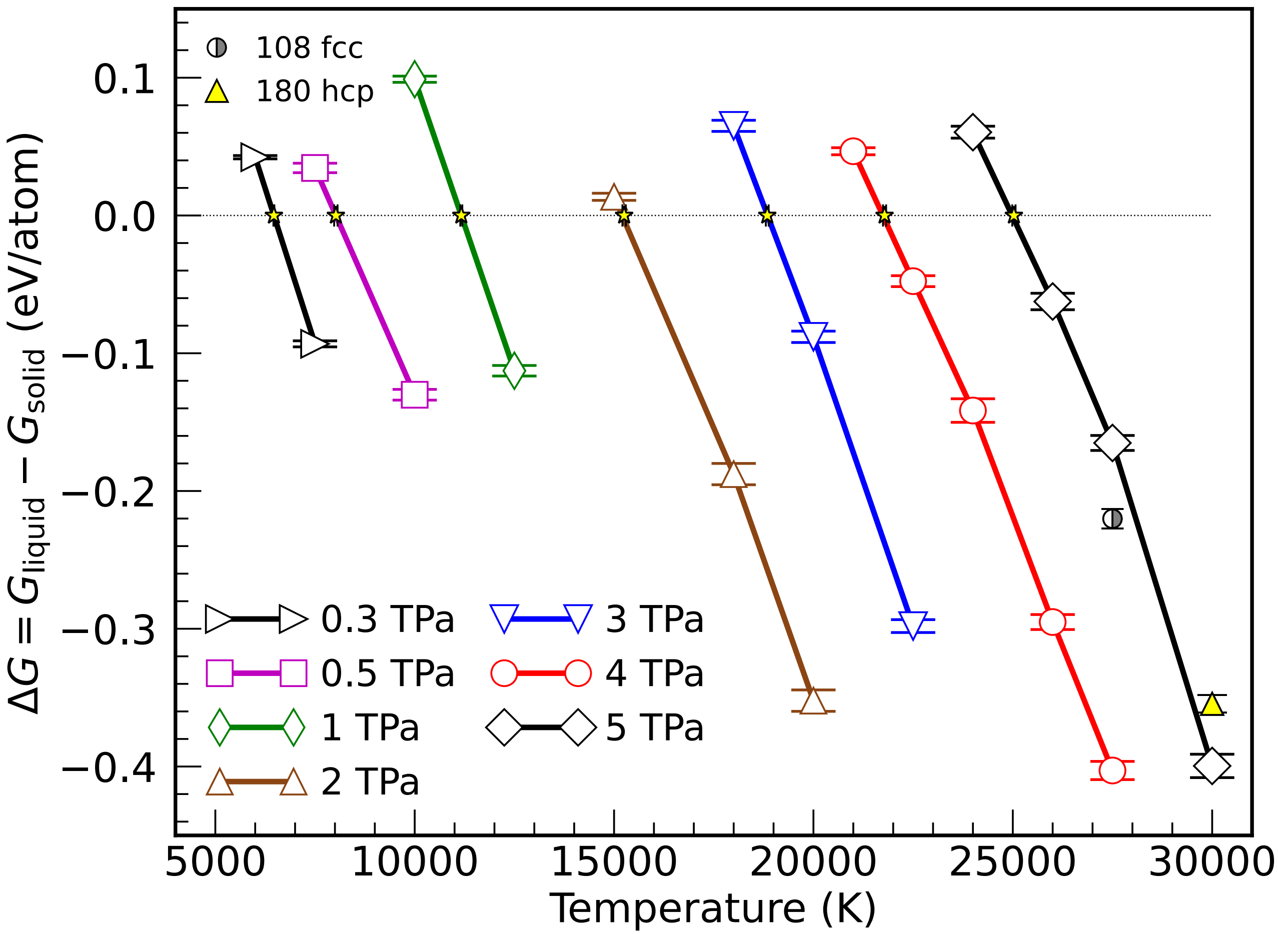
All filled symbols: Computer simulations

Experiments



Melting line of iron at 330 GPa informs about temperature in Earth's core, with caveats.

Derive melting temp from $G_{solid}(T_{melt},P)=G_{liquid}(T_{melt},P)$



Ab initio Free Energies with Thermodynamic Integration

For fixed NVT

$$F_B - F_A = \int_0^1 d\lambda \, \langle U_B - U_A \rangle_\lambda$$

$$U(\lambda) = U_A + \lambda(U_B - U_A)$$

Hybrid potential: $U(\lambda = 0) = U_A$ $U(\lambda = 1) = U_B$

$$G_{DFT} = F_{DFT} + P_{DFT}V$$

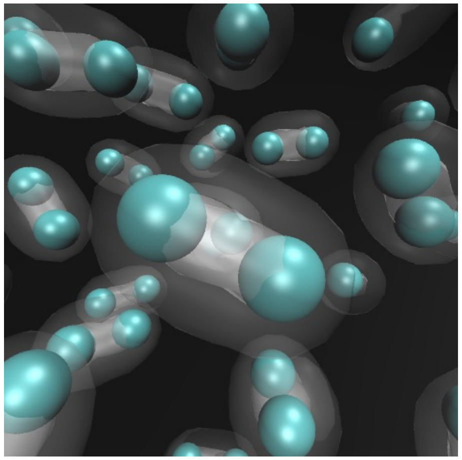
Gibbs free energy
(Which is more stable?)

$$TS_{DFT} = E_{DFT} - F_{DFT}$$

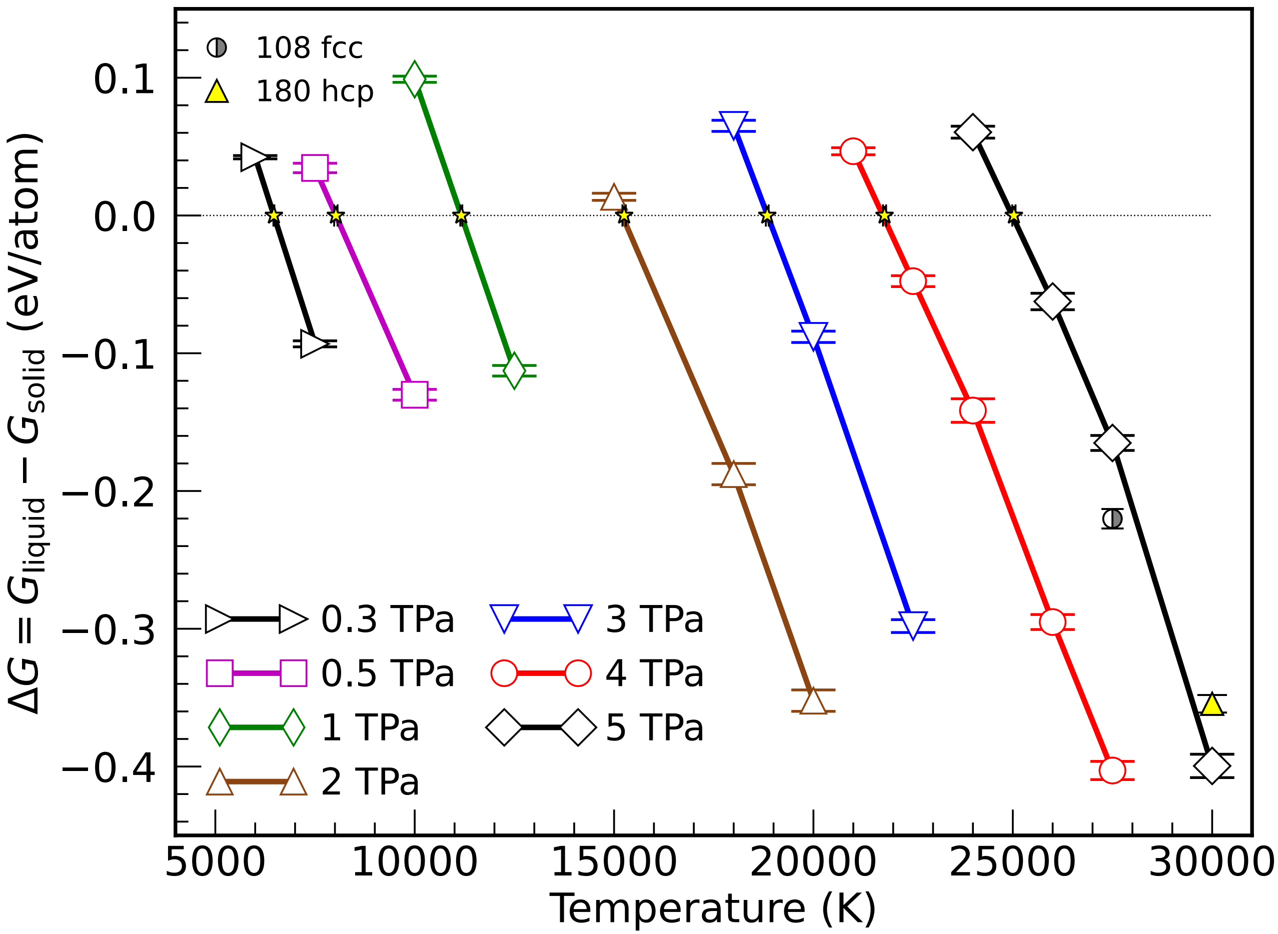
Entropy (ionic & electronic)
(Construct isentropes)

Solid: Einstein crystal → DFT

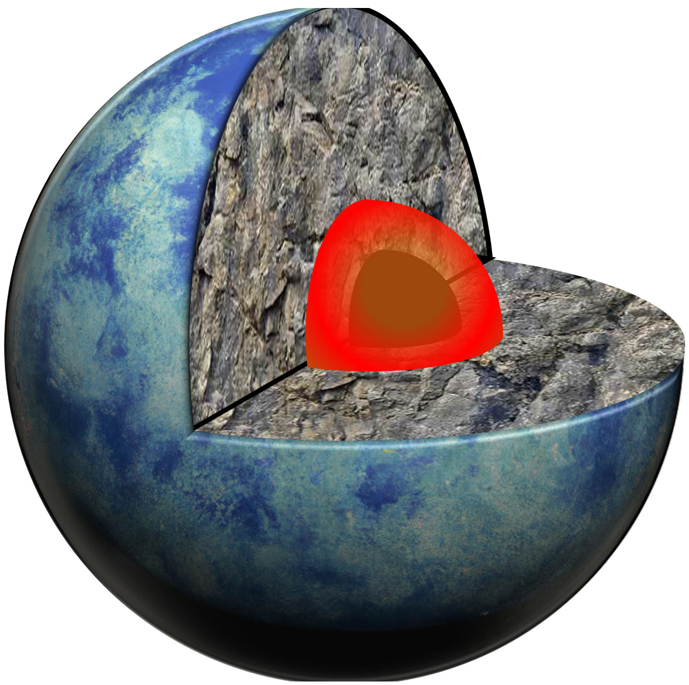
Liquid: Ideal gas → DFT

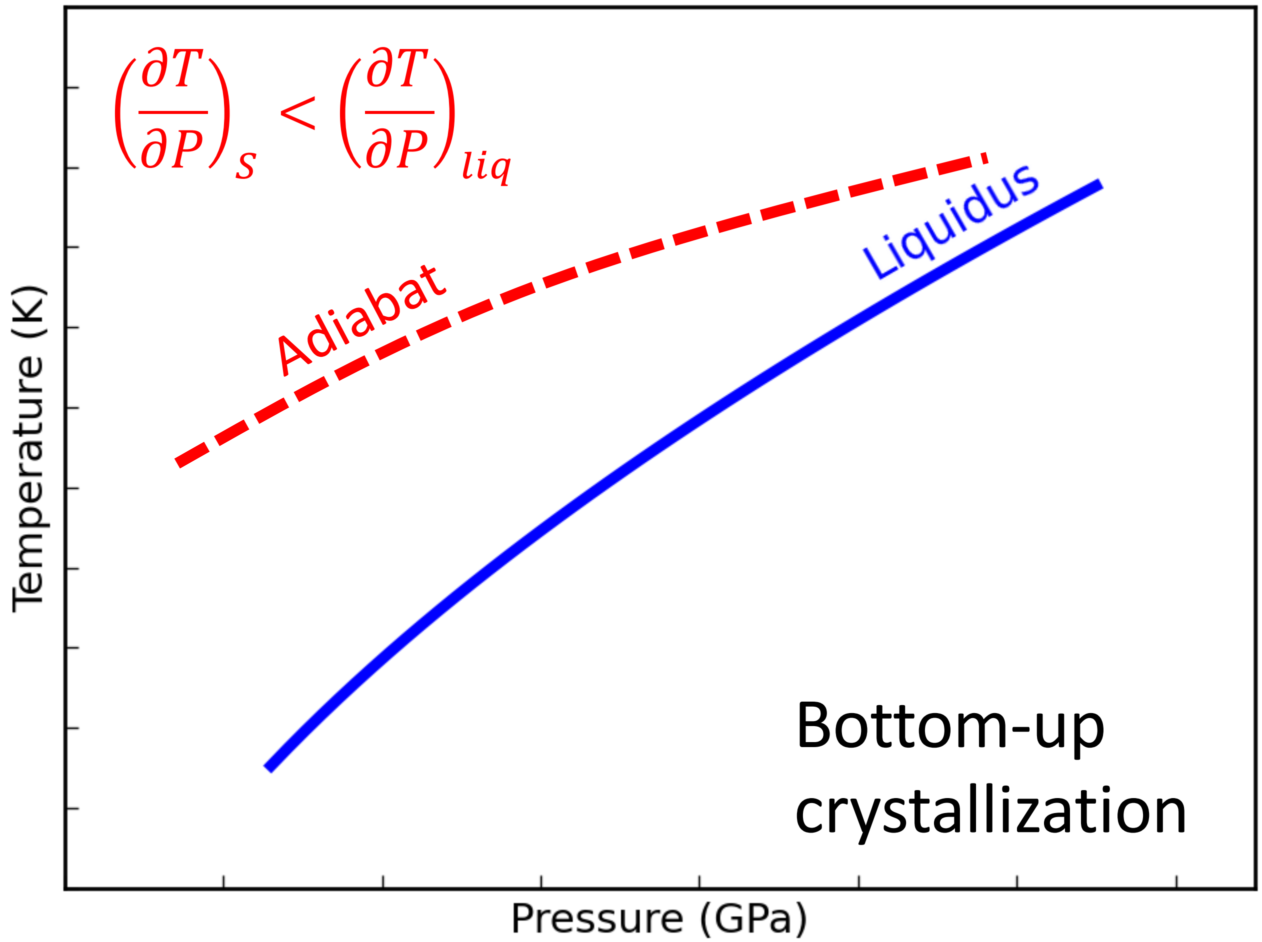


Derive melting temp from $G_{solid}(T_{melt},P)=G_{liquid}(T_{melt},P)$

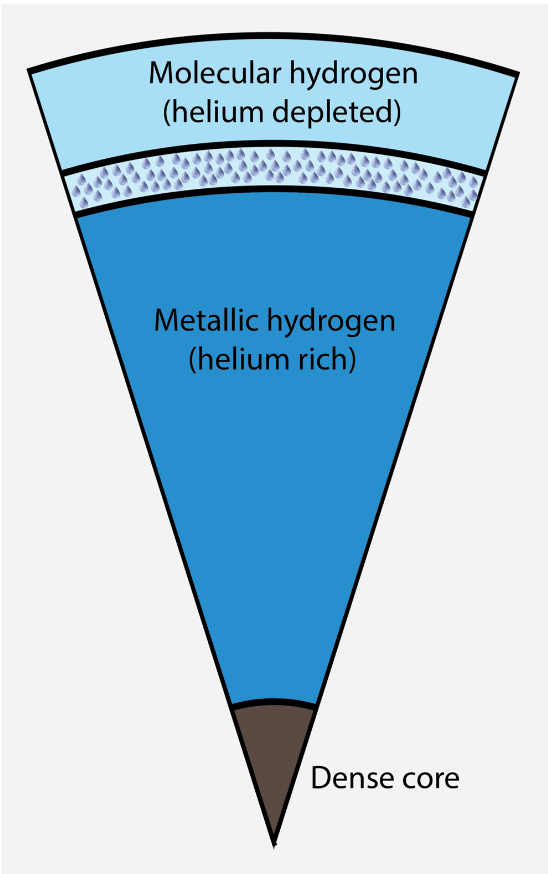


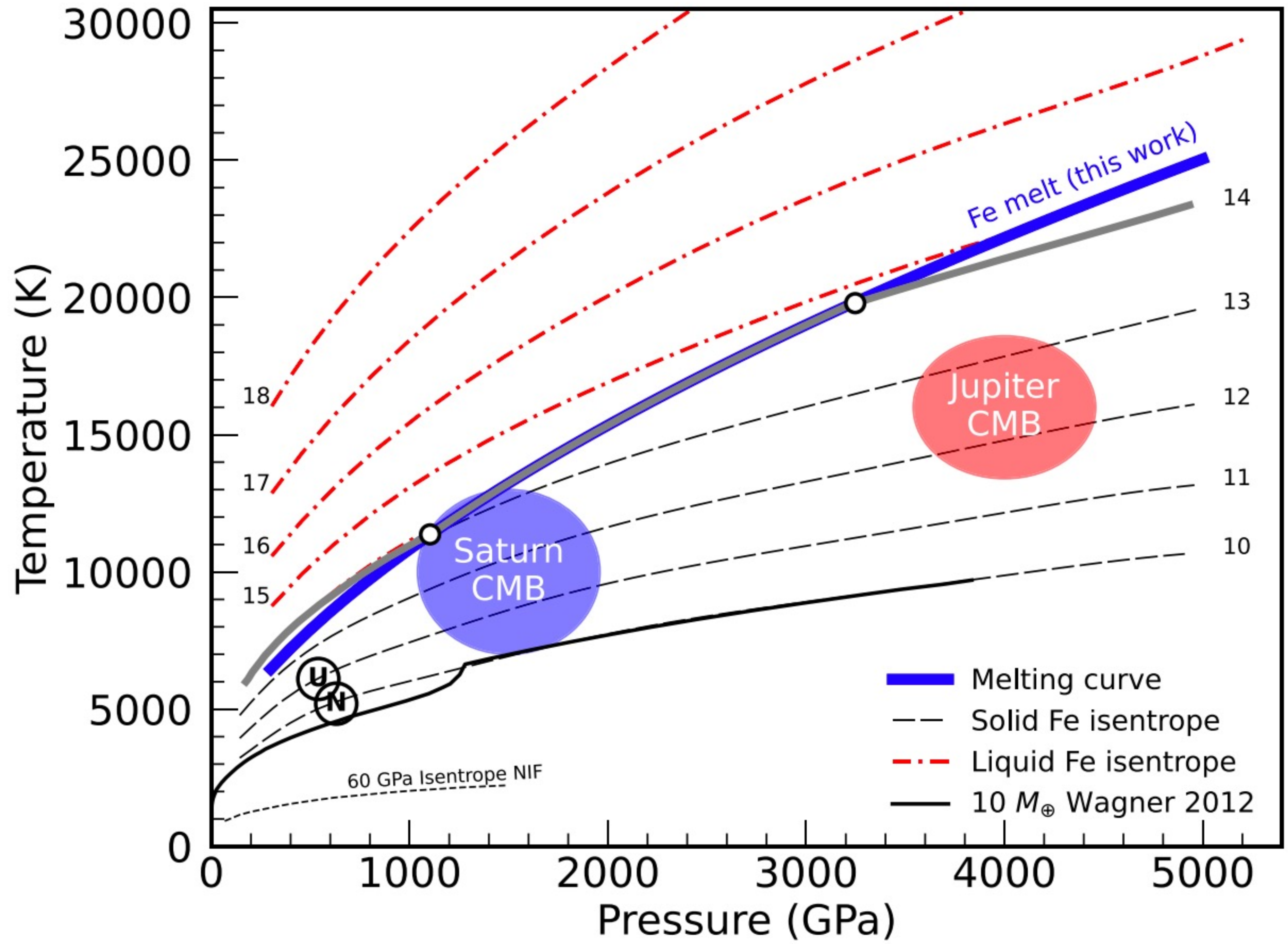
Iron cores of Super-Earths always crystallize from the center like in our Earth.





If Giant Planets are isentropic and had core of pure iron, they would be solid

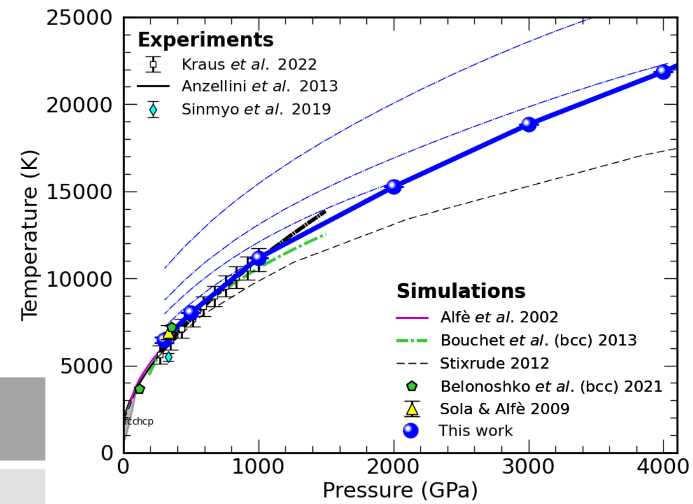




State of Core in Super-Earth Planets?

"The internal activity and thermal evolution of Earth-like planets," A. M. Papuc and G. F. Davies, Icarus 195, 447 (2008).

	<T> 2 ME	<T> 5 ME
Evolution begins	4300 K	5100 K
Temp after 10 Ga	3300 K	4300 K



Our melting line and planet model

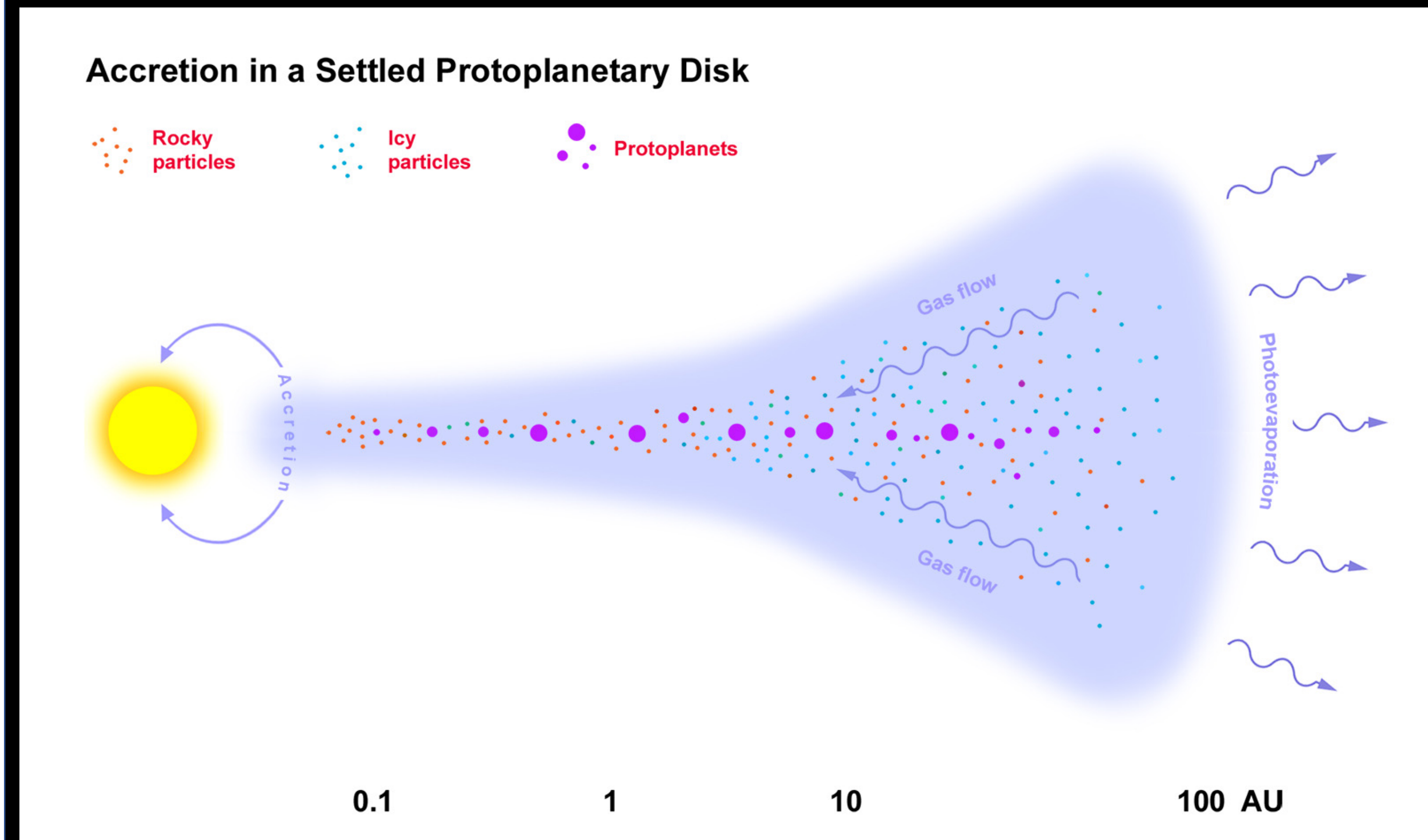
	<T> 2 ME	<T> 5 ME
Core cystall. starts with	8070 K	12500 K
And ends when	7410 K	10650 K

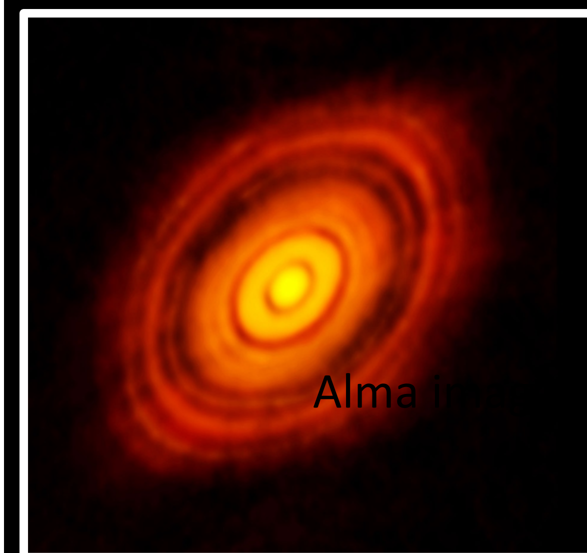
For all published models, the cores of Super-Earth planet would be frozen. So, no magnetic field. Implications for life? One exception Boujibar et al. (Wide range of primordial heat, solid and liquid core possible.

Part II

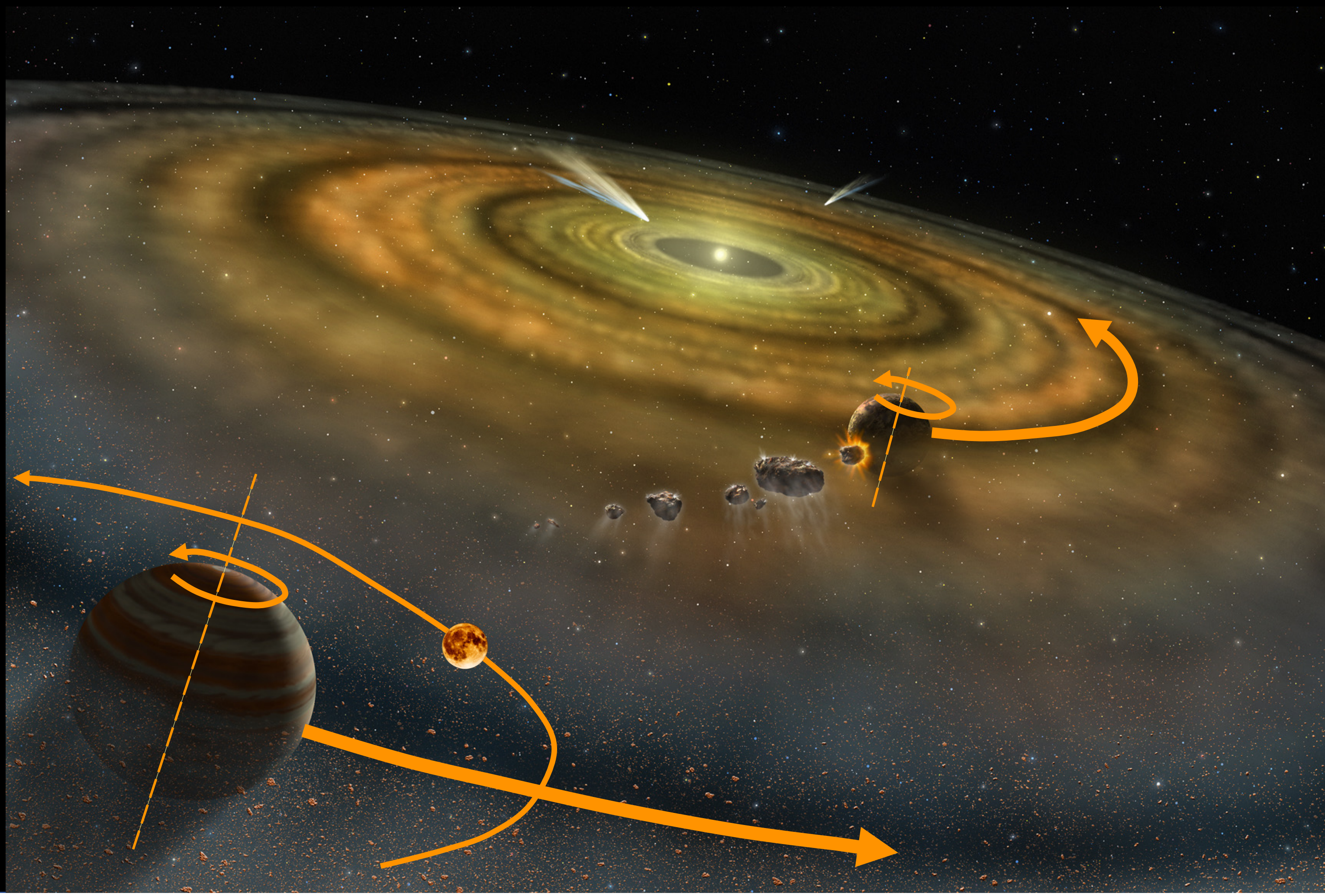
2. How do planets and moons moves in our solar system? (Counterclockwise)

Solar Systems Form From a Disk of Gas and Dust

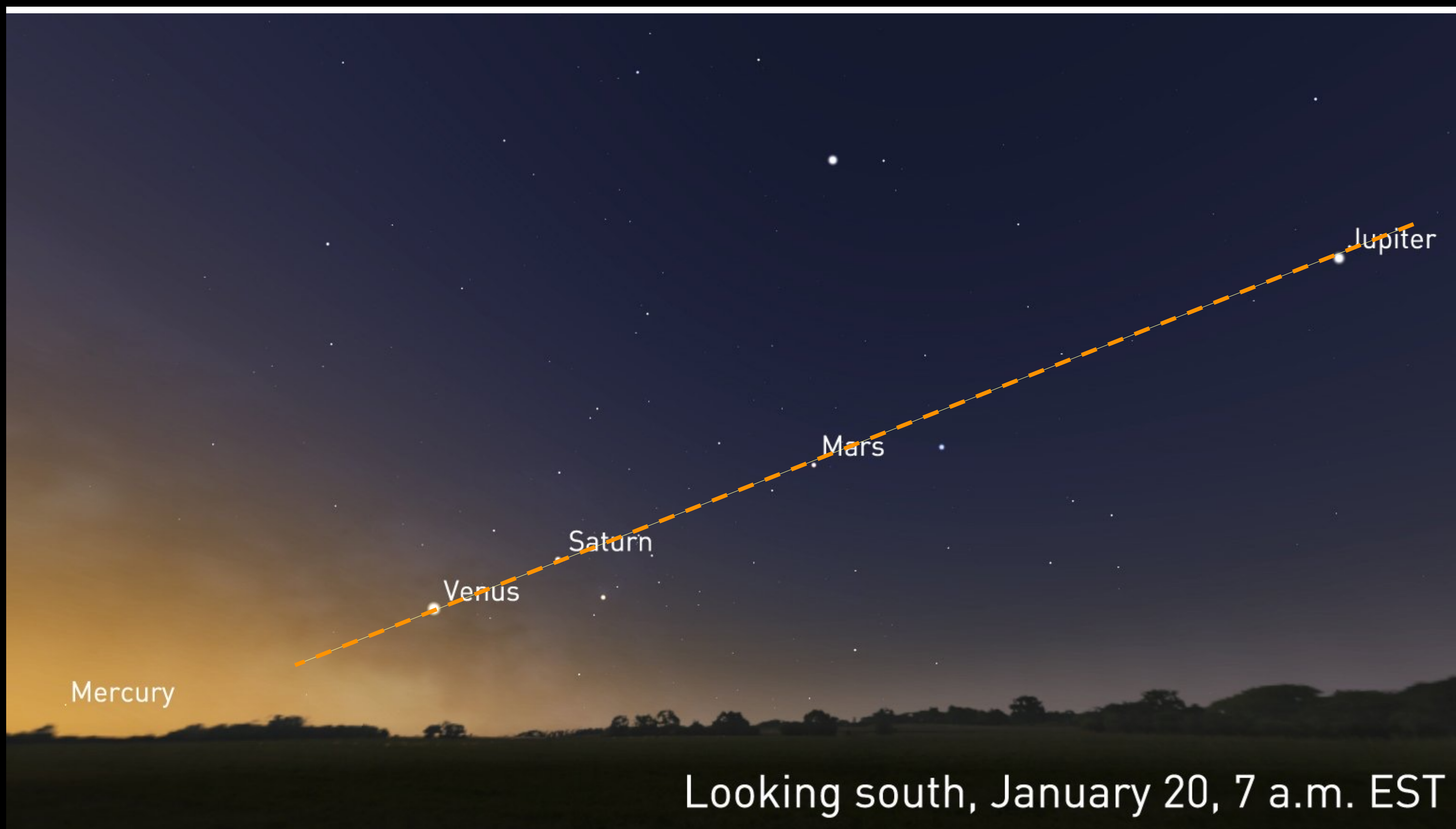




Solar Systems Form From a Disk of Gas and Dust



All Planets Orbit the Sun in one Plane in Counterclockwise Direction



How does our Moon Move through the Night's Sky?

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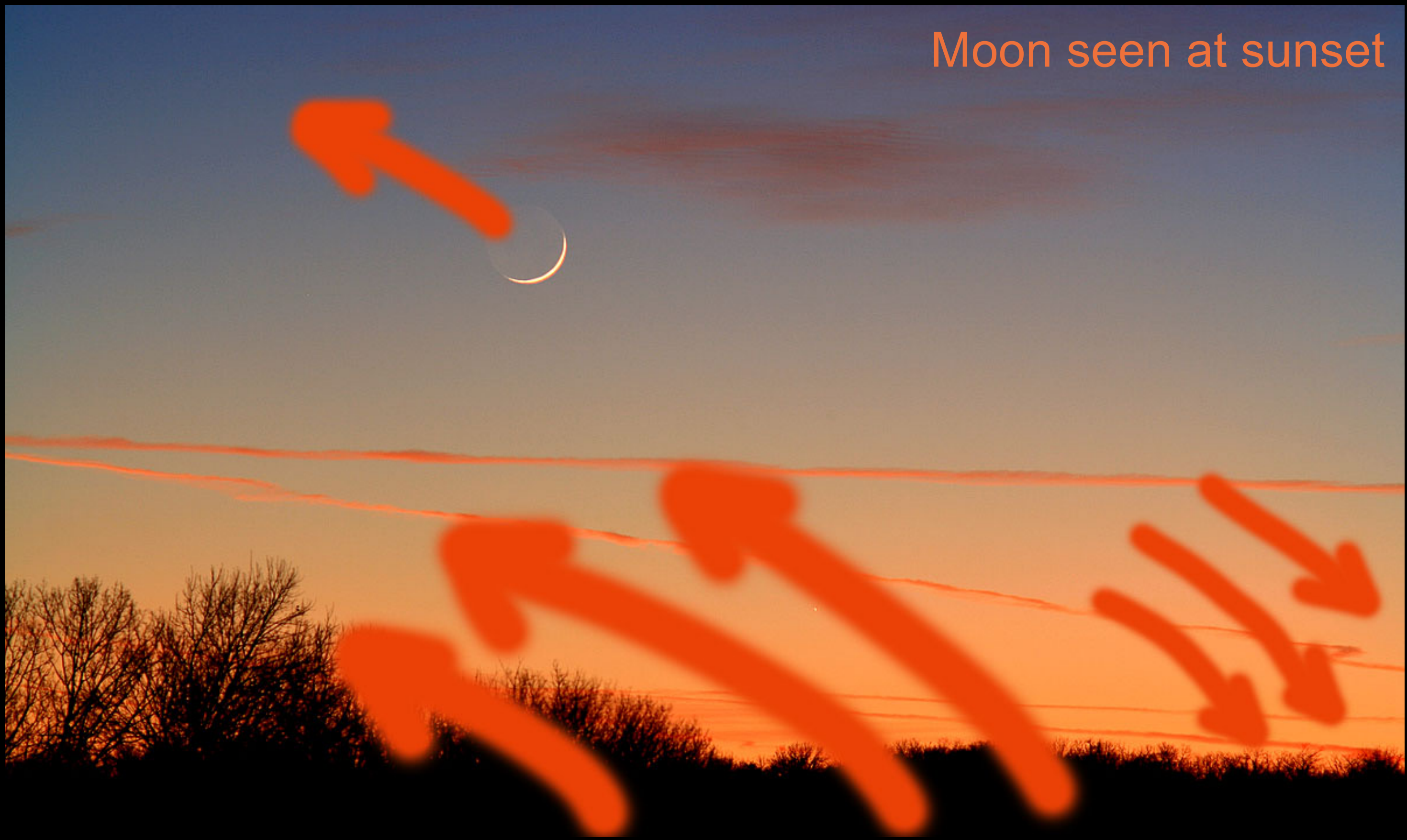
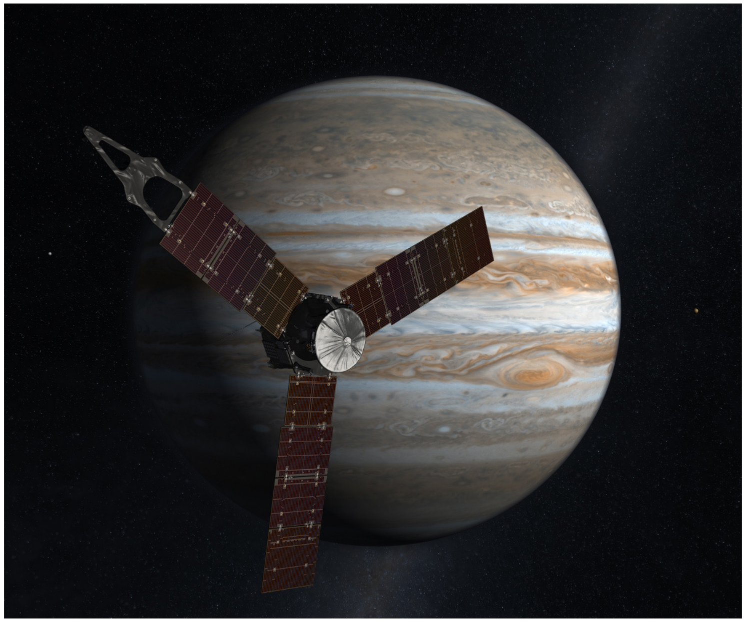


Part 4

4. Juno Mission to Jupiter

Juno Mission launched successfully August 2011

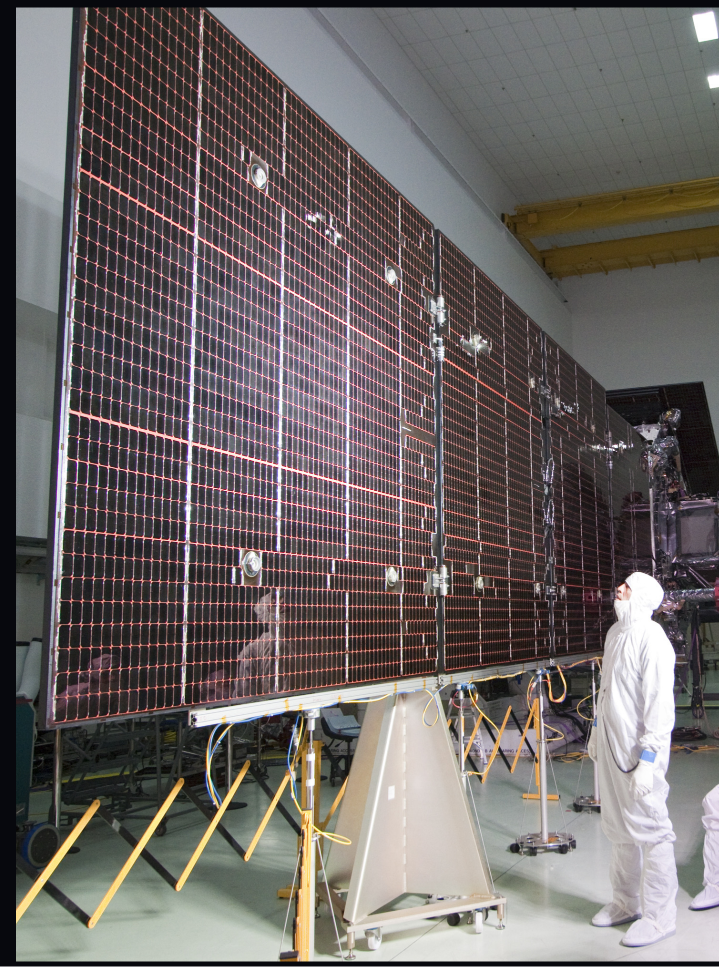
My contribution:
- **Equation of state calculations for hydrogen-helium mixtures**
- **Models for the planet's interior**



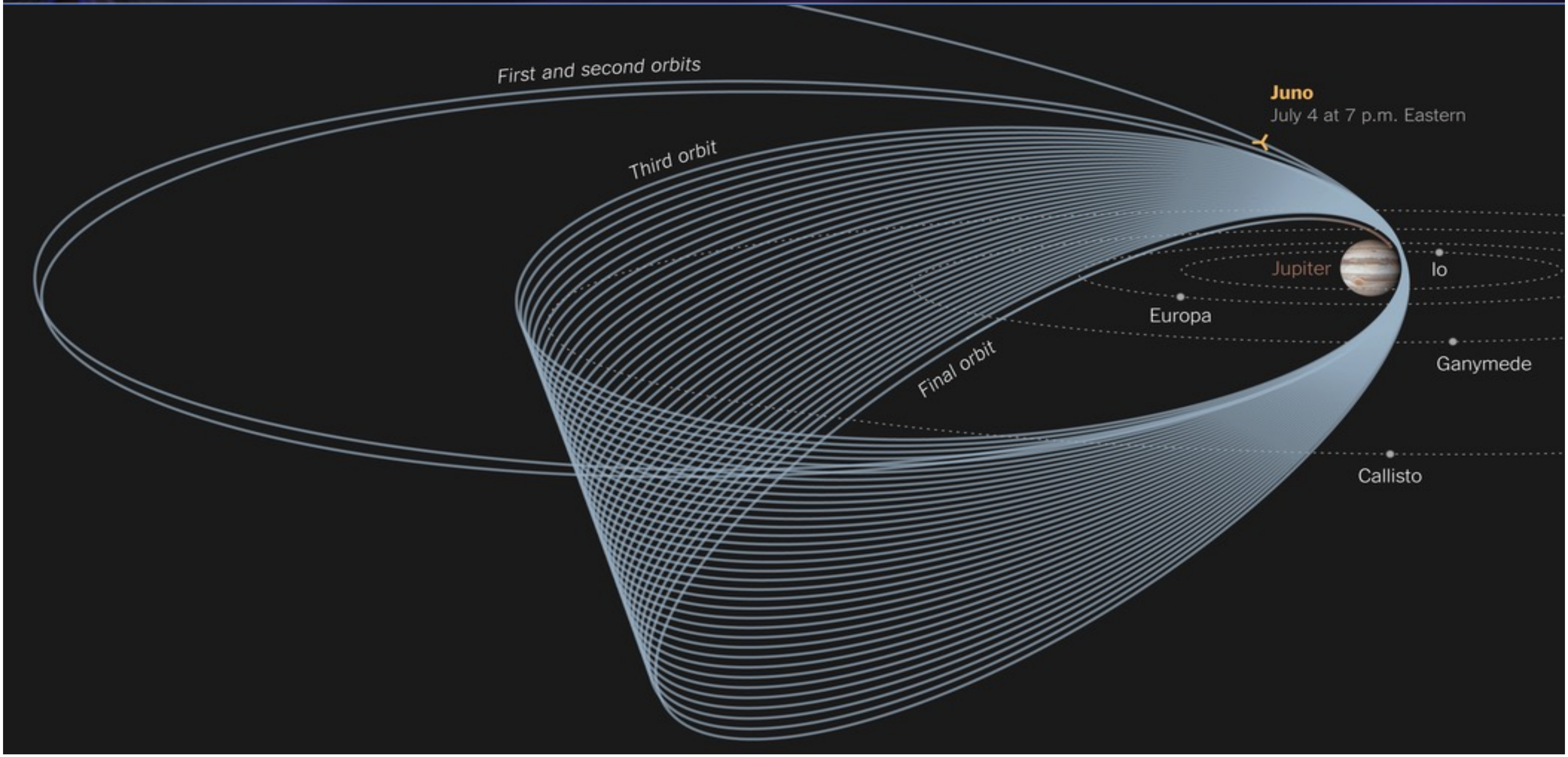
Mission Timeline:
- **Launch - August 2011**
- **Earth flyby gravity assist - October 2013**
- **Jupiter arrival - July 2016**
- **Mission extended in 2022**

Juno's solar panels – its only source of energy.

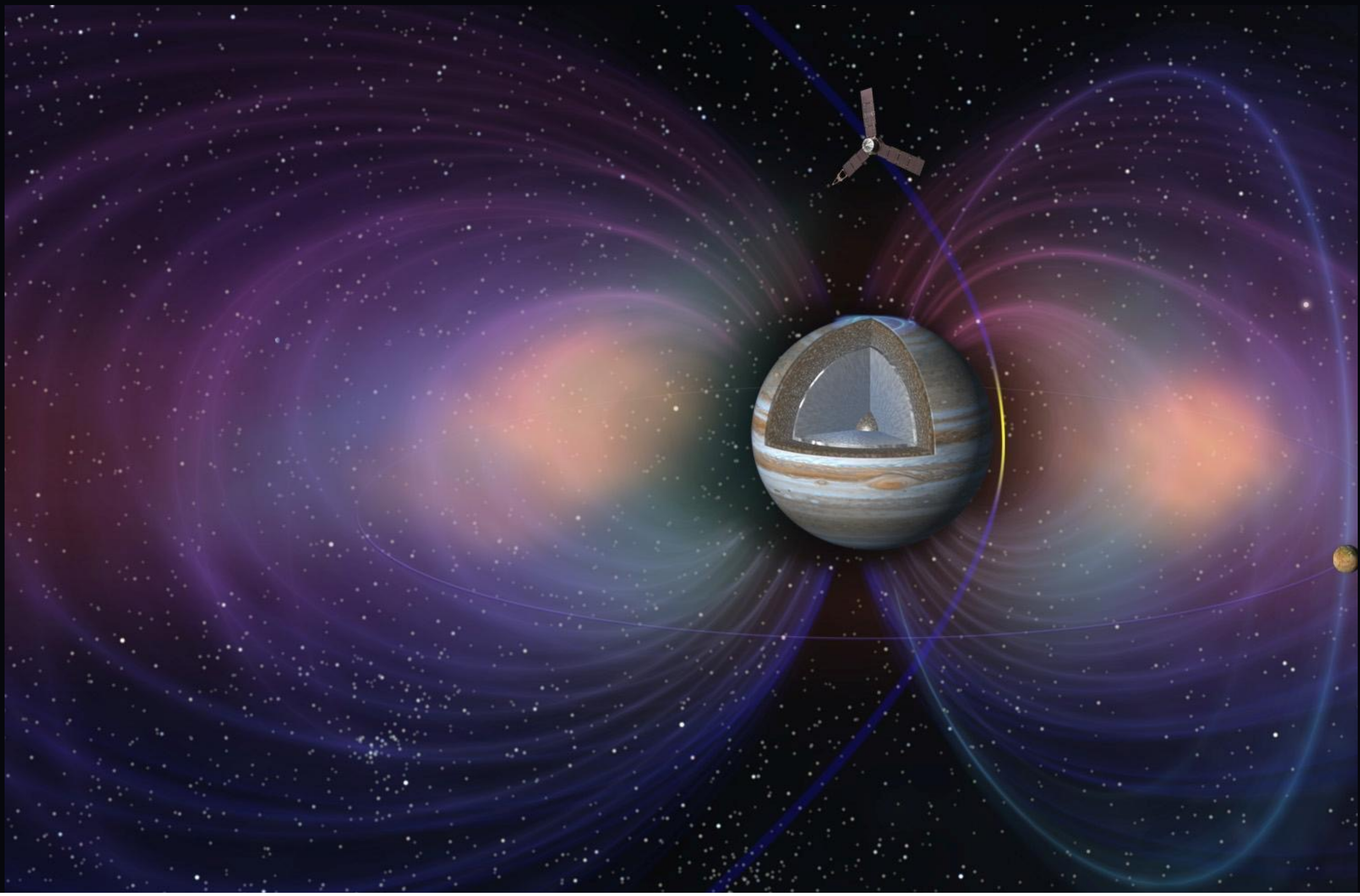
(No nuclear power source on board.)



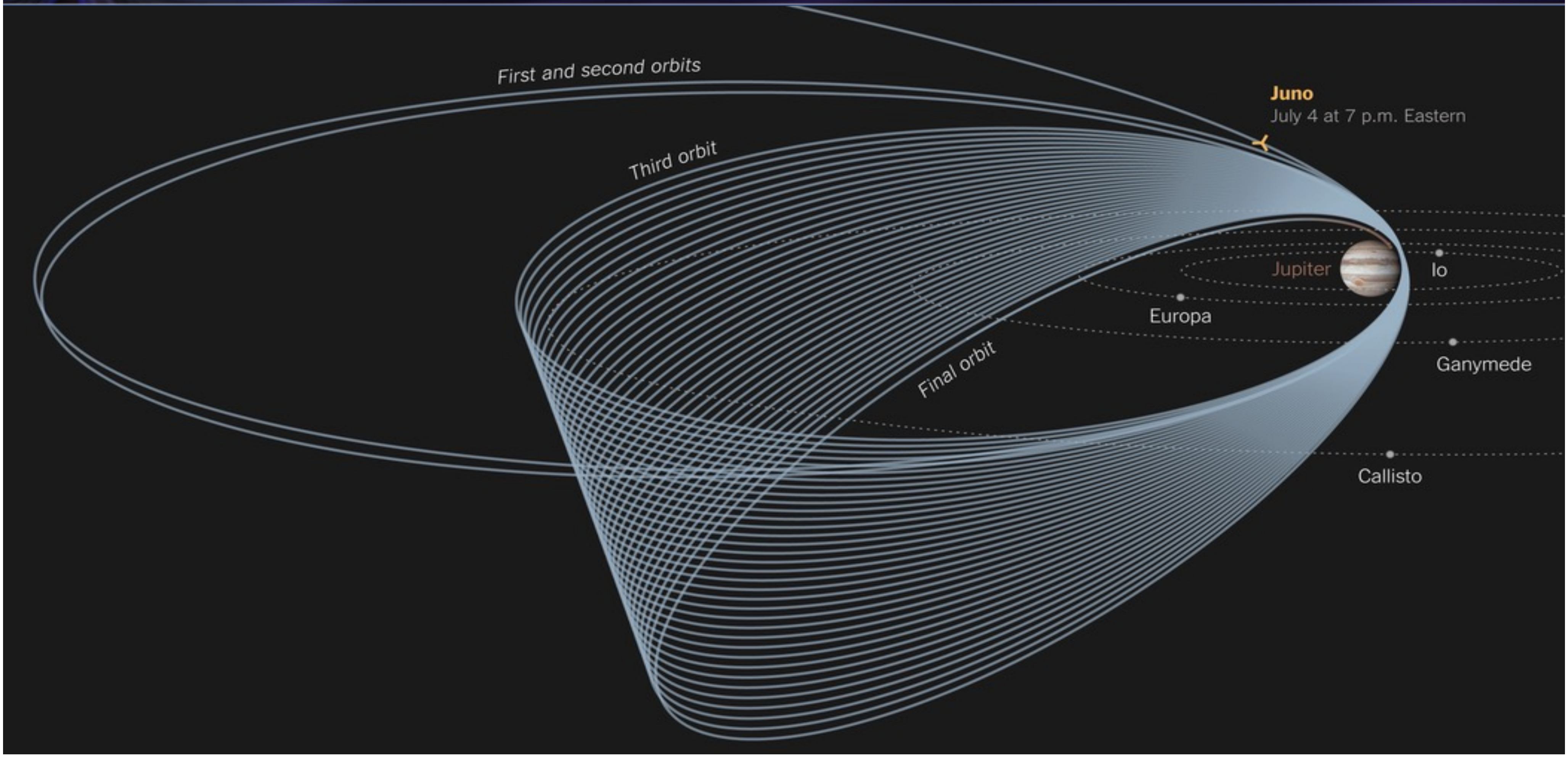
Juno's low-periapse orbits



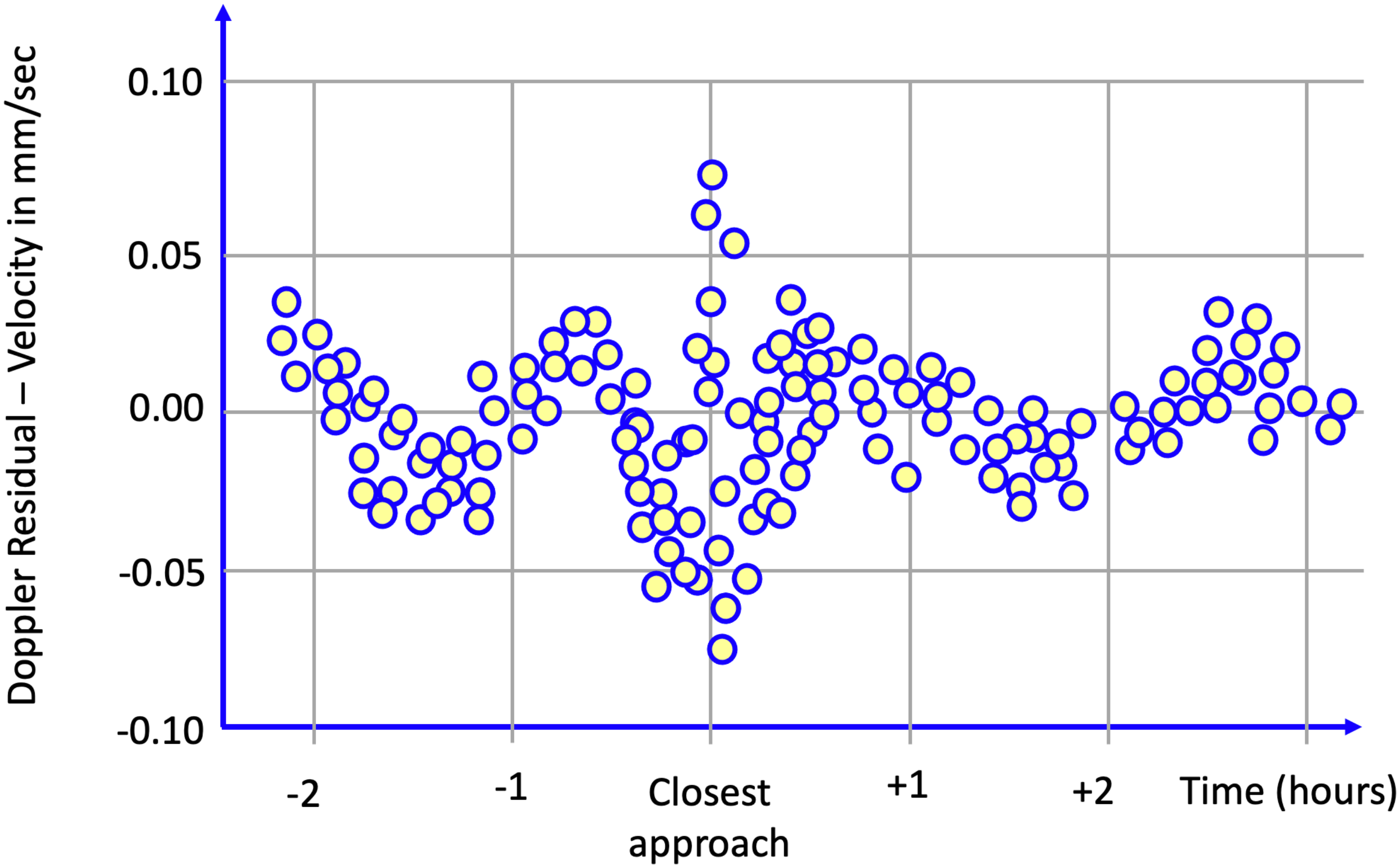
Juno’s low-periapse orbits



Juno’s low-periapse orbits

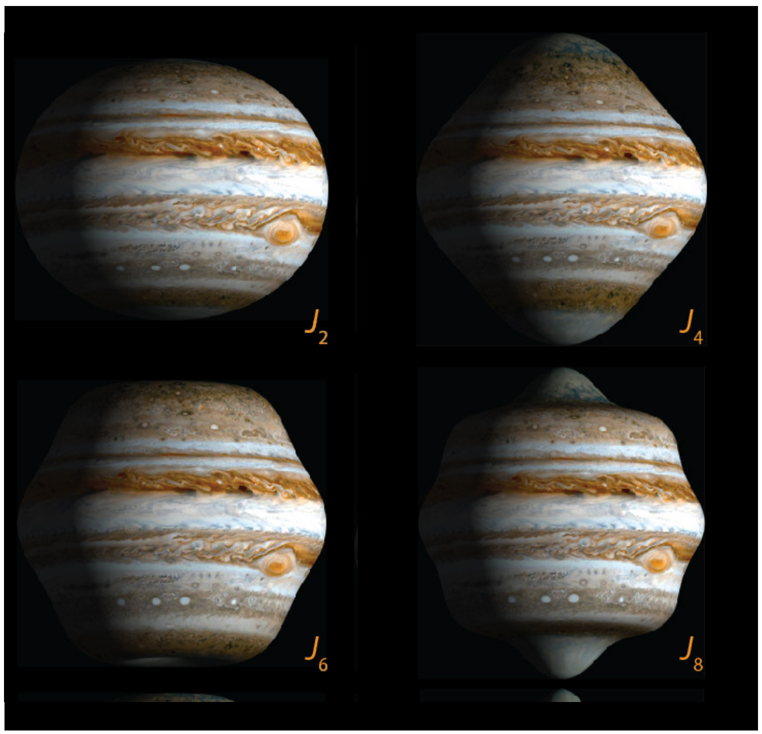


Processing the Doppler Signal from Spacecraft



Measured Gravity Field

$$V(r,\mu) = \frac{GM}{r}\left[1 - \sum_{n=1}^{\infty}\left(\frac{a}{r}\right)^{2n} J_{2n} P_{2n}(\mu)\right]$$



Measurements

Pioneer and Voyager spacecrafts

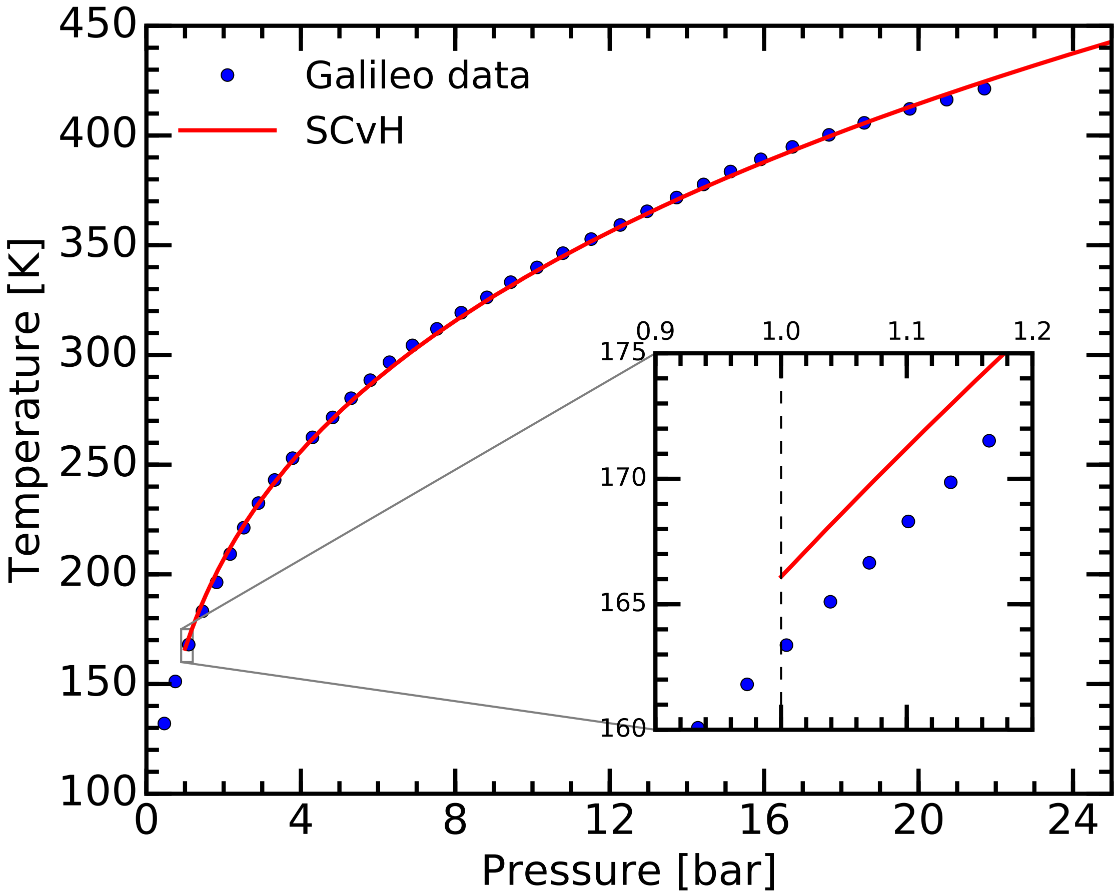
$$J_2 = 14697 \pm 1$$
$$J_4 = -584 \pm 5$$
$$J_6 = 31 \pm 20$$

Measurements of Juno orbiter

$$J_2 = 14696.5735 \pm 0.0017$$
$$J_4 = -586.6085 \pm 0.0024$$
$$J_6 = 34.2007 \pm 0.0067$$

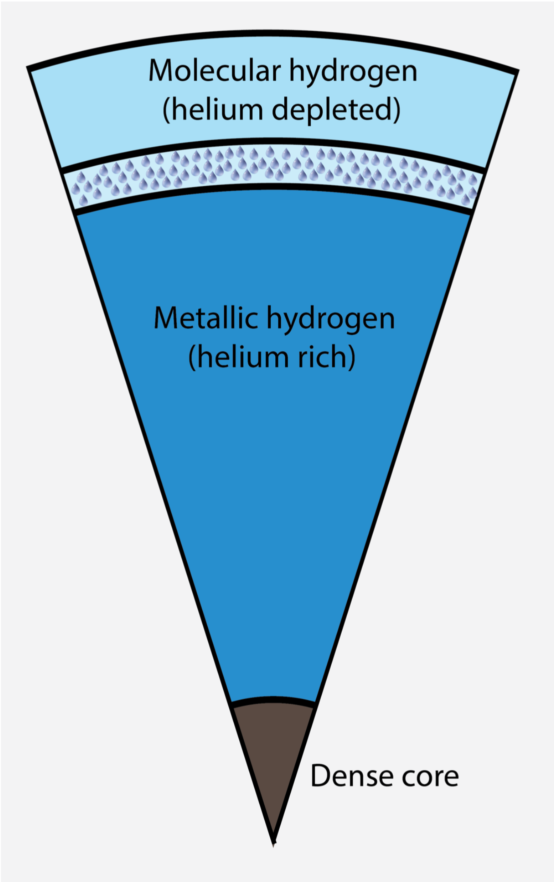
Inverse problem: Use gravity measurement to infer properties of interior.

The Galileo Entry Probe Measure the Temperature of Jupiter's Atmosphere but only Survived for 78 Minutes

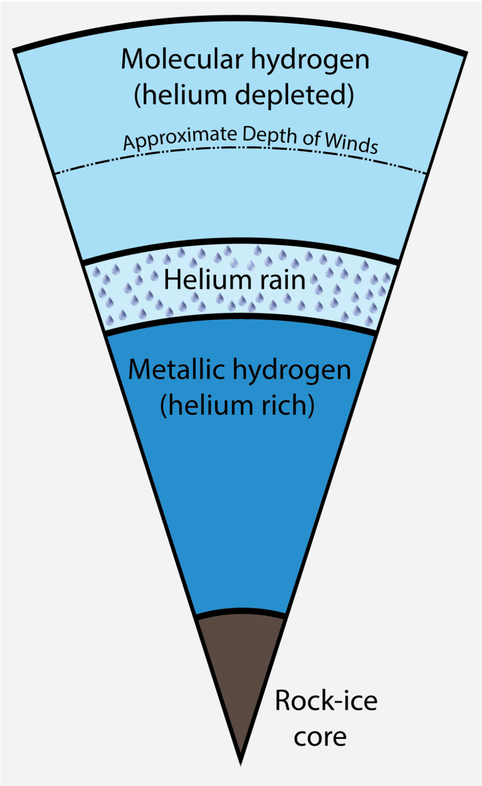


- We use our *ab initio* EOS (MH13) for P>5 GPa
- SC EOS for P<5 GPa anchored to T_{1bar}=166.1 K and S_{mol}=7.078061 k_b/el.

Traditional 4-layer Models for Saturn and Jupiter

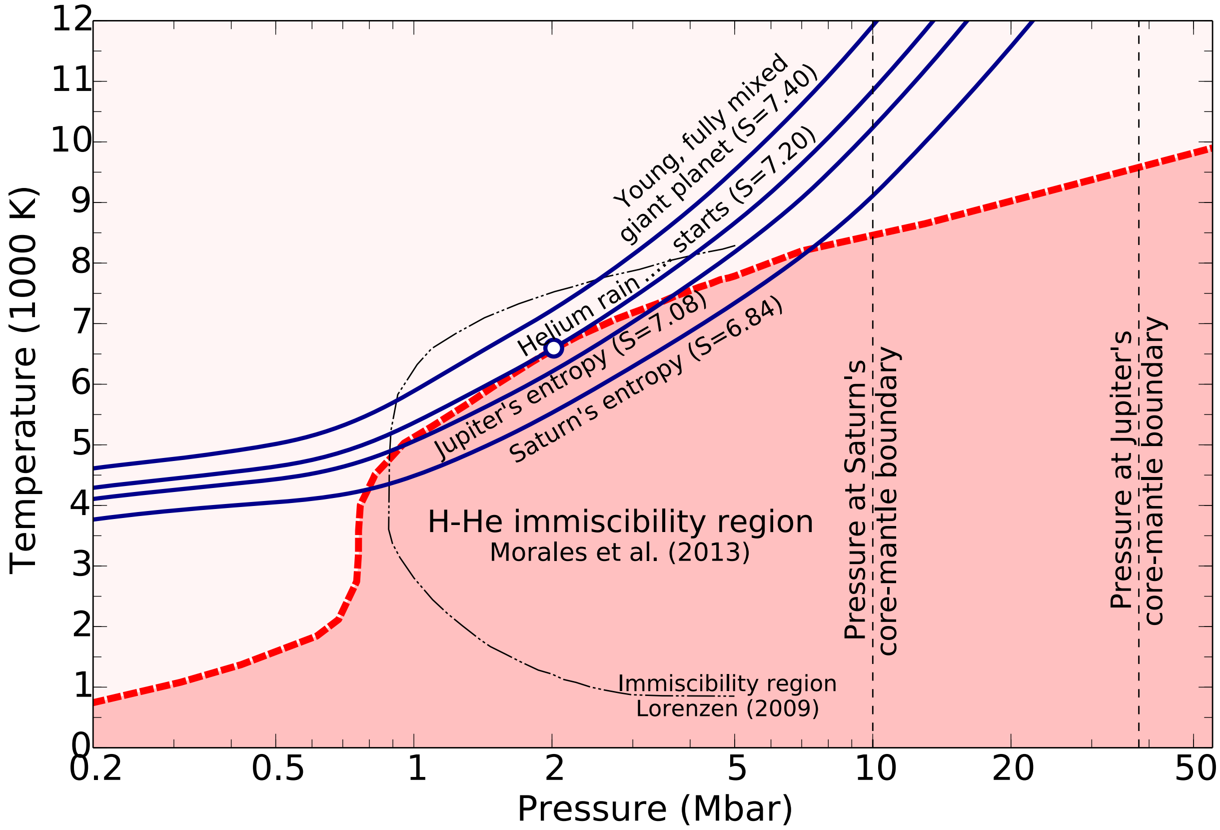


Jupiter's interior



Saturn's interior

Planets cool convectively: So we assume most of their interior layers are isentropic and homogeneous



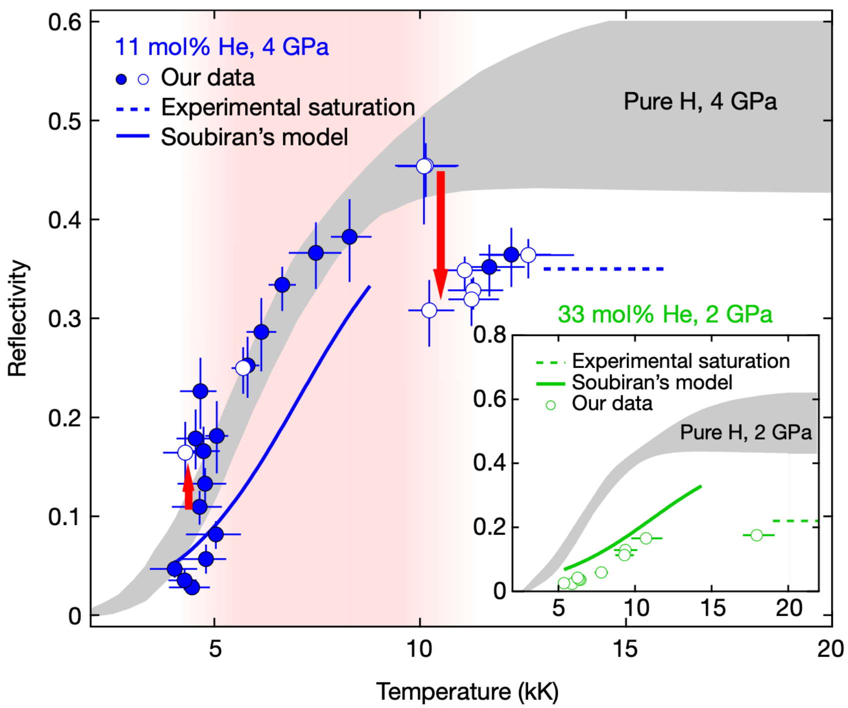
One enjoyable way to observe convection: Ordering miso soup in a sushi restaurant

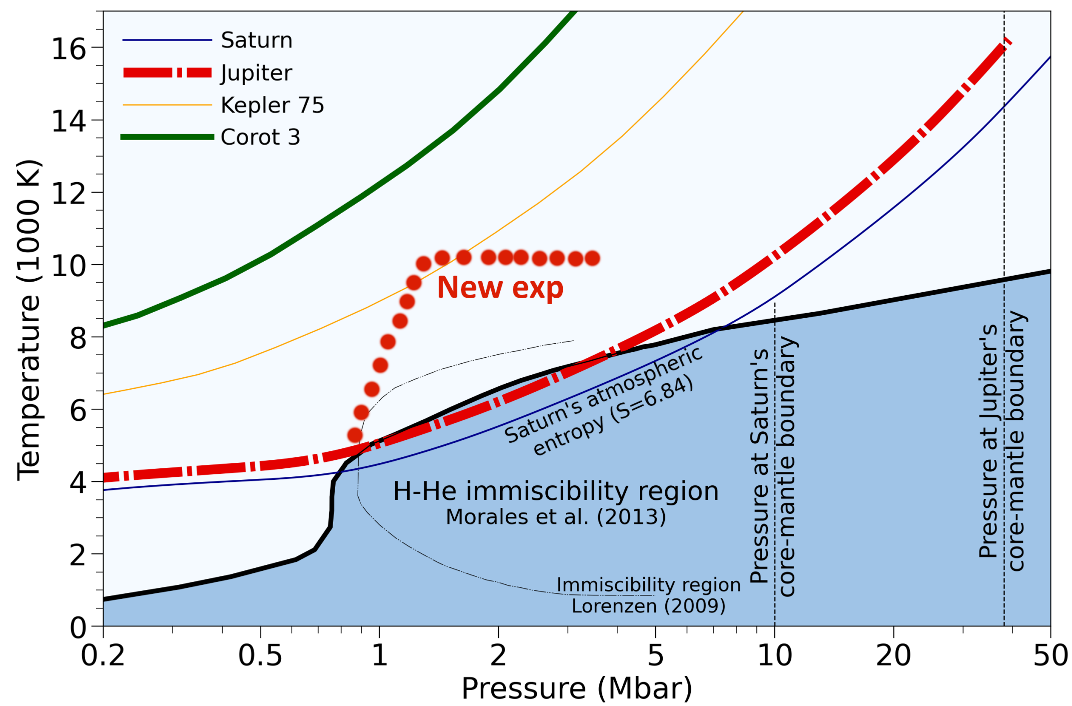
Evidence of hydrogen–helium immiscibility at Jupiter-interior conditions

https://doi.org/10.1038/s41586-021-03516-0

Received: 13 October 2015

S. Brygoo[1]✉, P. Loubeyre[1]✉, M. Millot[2], J. R. Rygg[3], P. M. Celliers[2], J. H. Eggert[2], R. Jeanloz[4] & G. W. Collins[3]

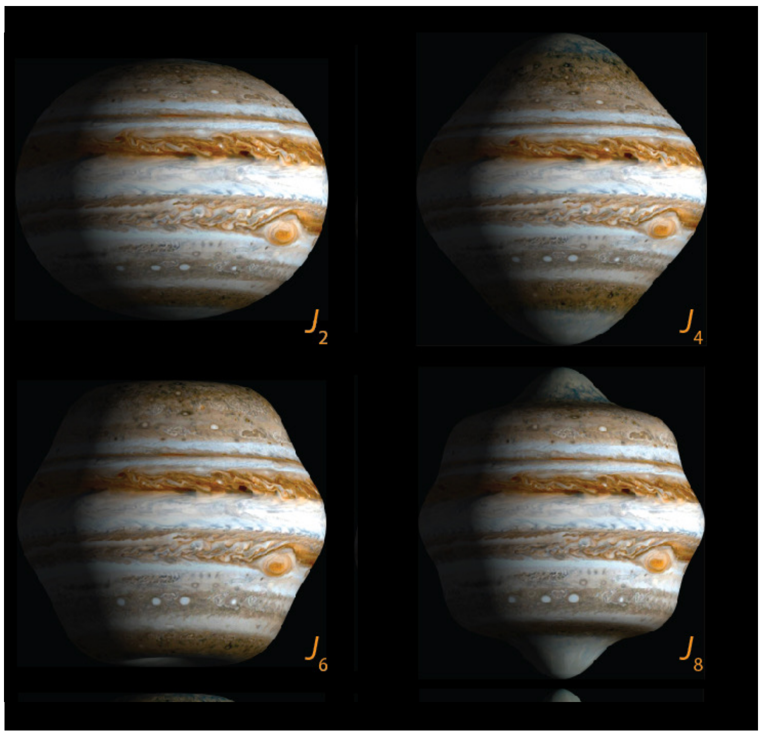




Measured Gravity Field

Interior Models

$$V(r,\mu) = \frac{GM}{r}\left[1 - \sum_{n=1}^{\infty}\left(\frac{a}{r}\right)^{2n} J_{2n} P_{2n}(\mu)\right]$$

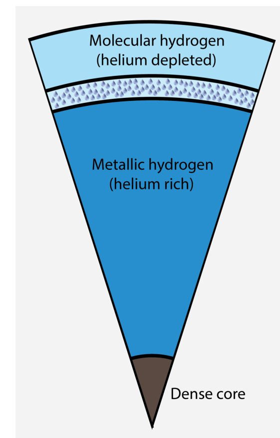


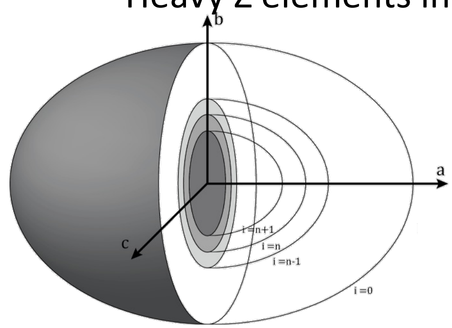
Match: M, R, gravity moments J_{2n}

$$J_n = -\frac{2\pi}{Ma^n}\int_{-1}^{1} d\mu \int_{0}^{a} r^{n+2} P_n(\mu)\,\rho\,(r,\mu)\,dr$$

Model parameters:

- EOS of H, He, Z (from *ab initio* simulations)
- Size of the core
- How much helium was sequestered
- Interior entropy
- Heavy Z elements in metallic H
- Heavy Z elements in molecular H





Bill Hubbard's CMS method.

Concentric Maclaurin Spheroid Method, Hubbard, ApJ (2013)
Accelerated CMS method Militzer et al, ApJ (2019)

Measured Gravity Field

Interior Models

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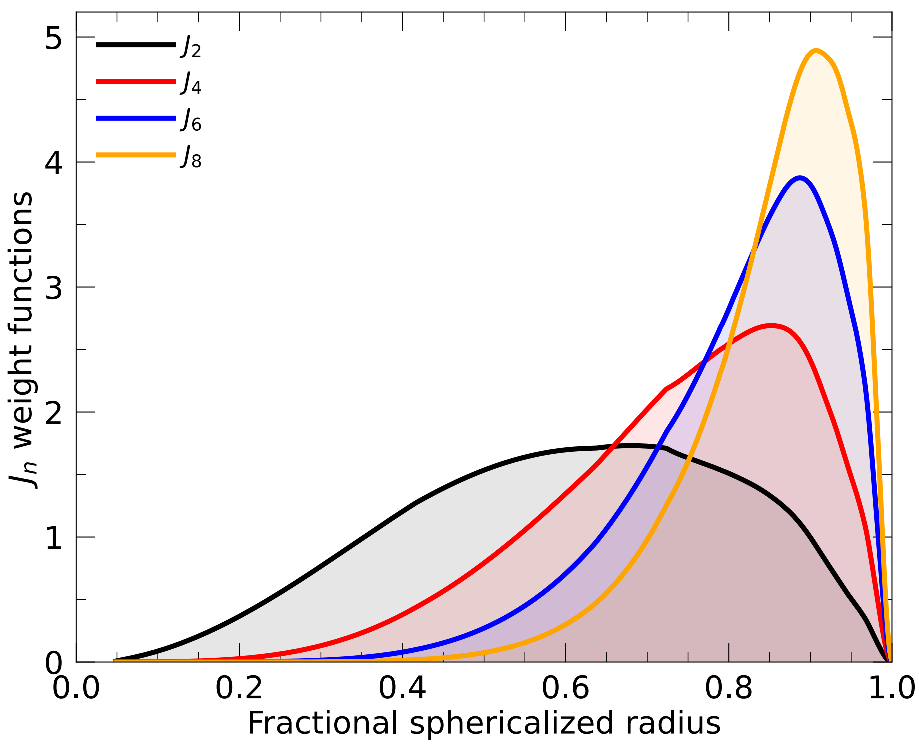

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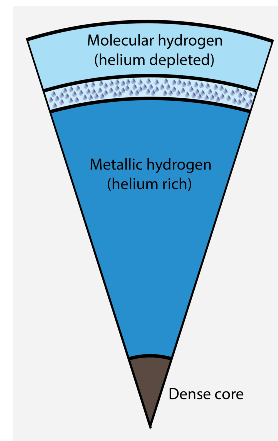
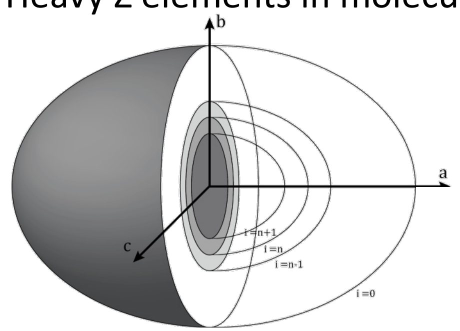


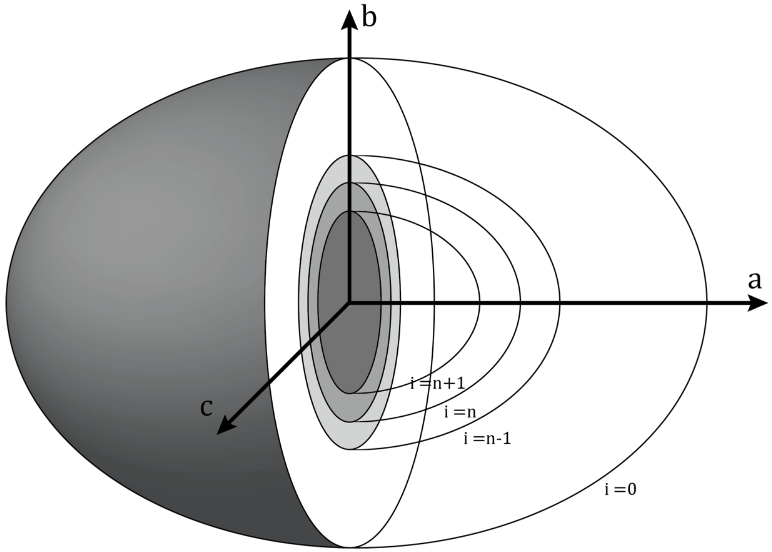


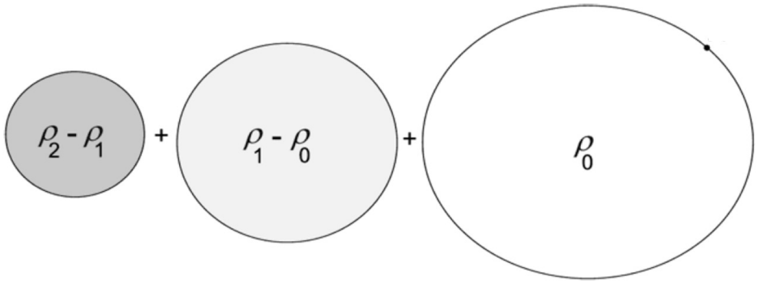
Bill Hubbard's CMS method.

Concentric Maclaurin Spheroid (CMS) theory for rotating bodies

<u>Model parameters:</u>

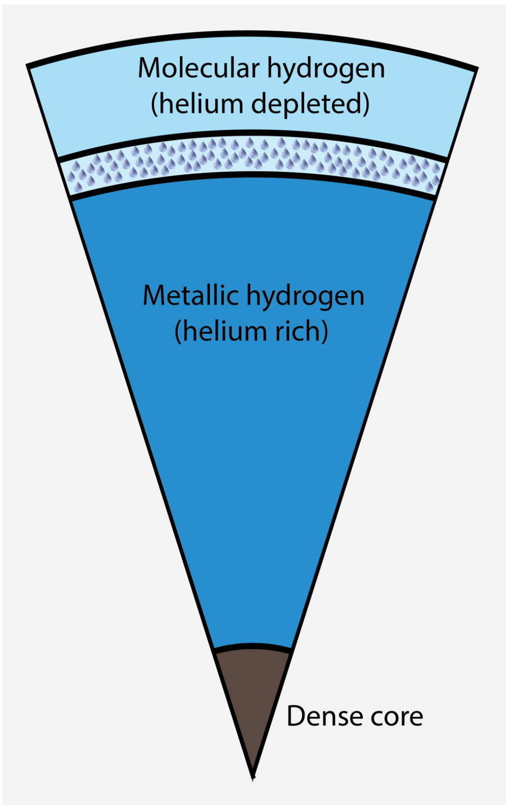
- EOS of H, He, Z (from *ab initio* simulations)
- Size of the core
- How much helium was sequestered
- Interior entropy
- Heavy Z elements in metallic H
- Heavy Z elements in molecular H

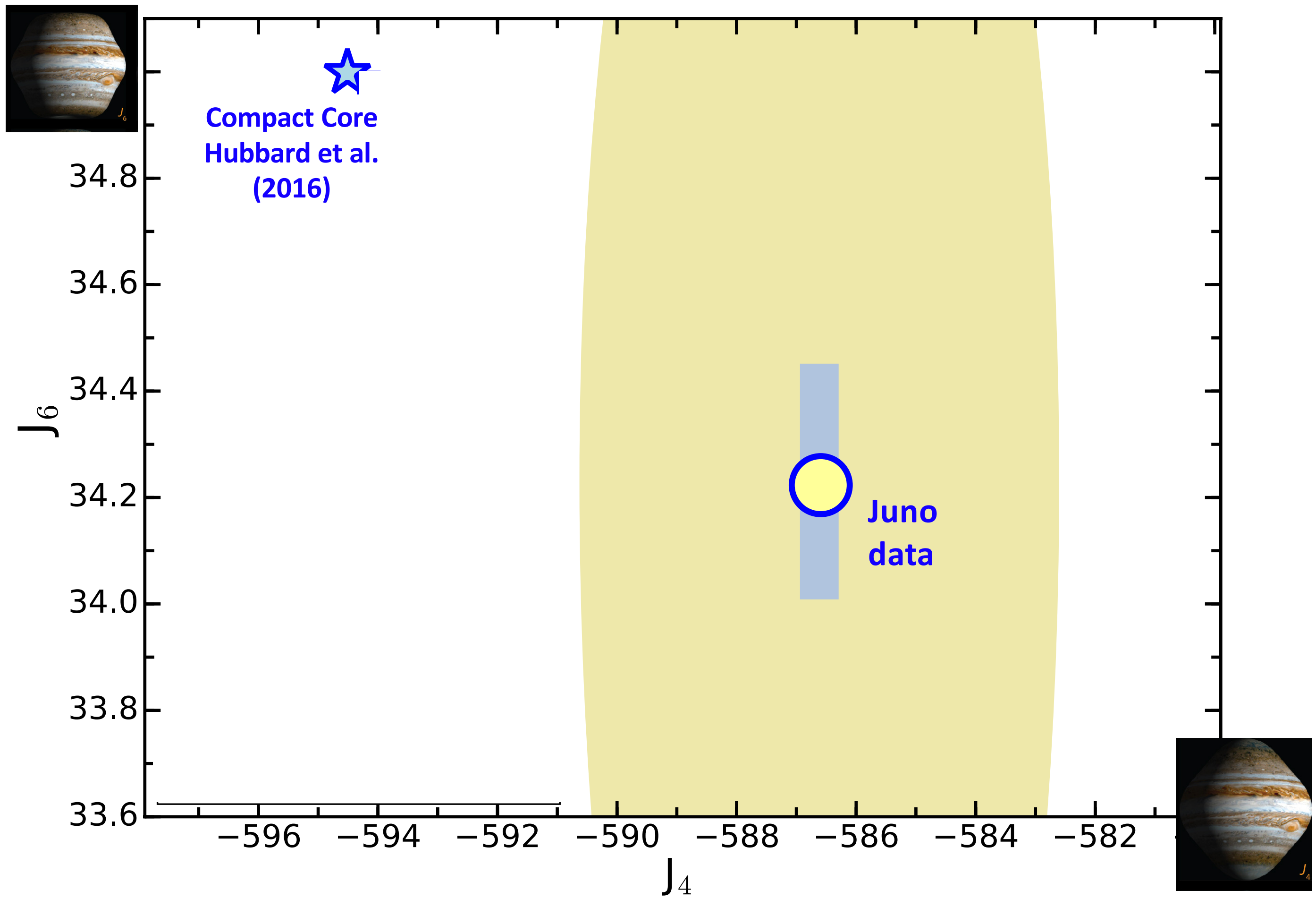




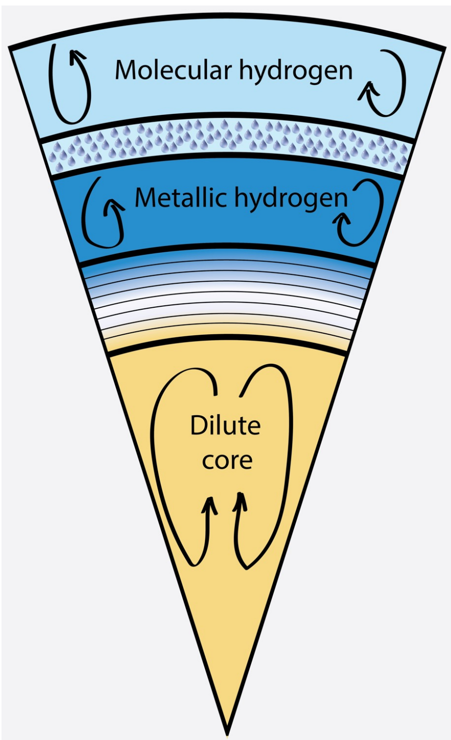
Concentric Maclaurin Spheroid Method, Hubbard, ApJ (2013)
Accelerated CMS method Militzer et al, ApJ (2019)

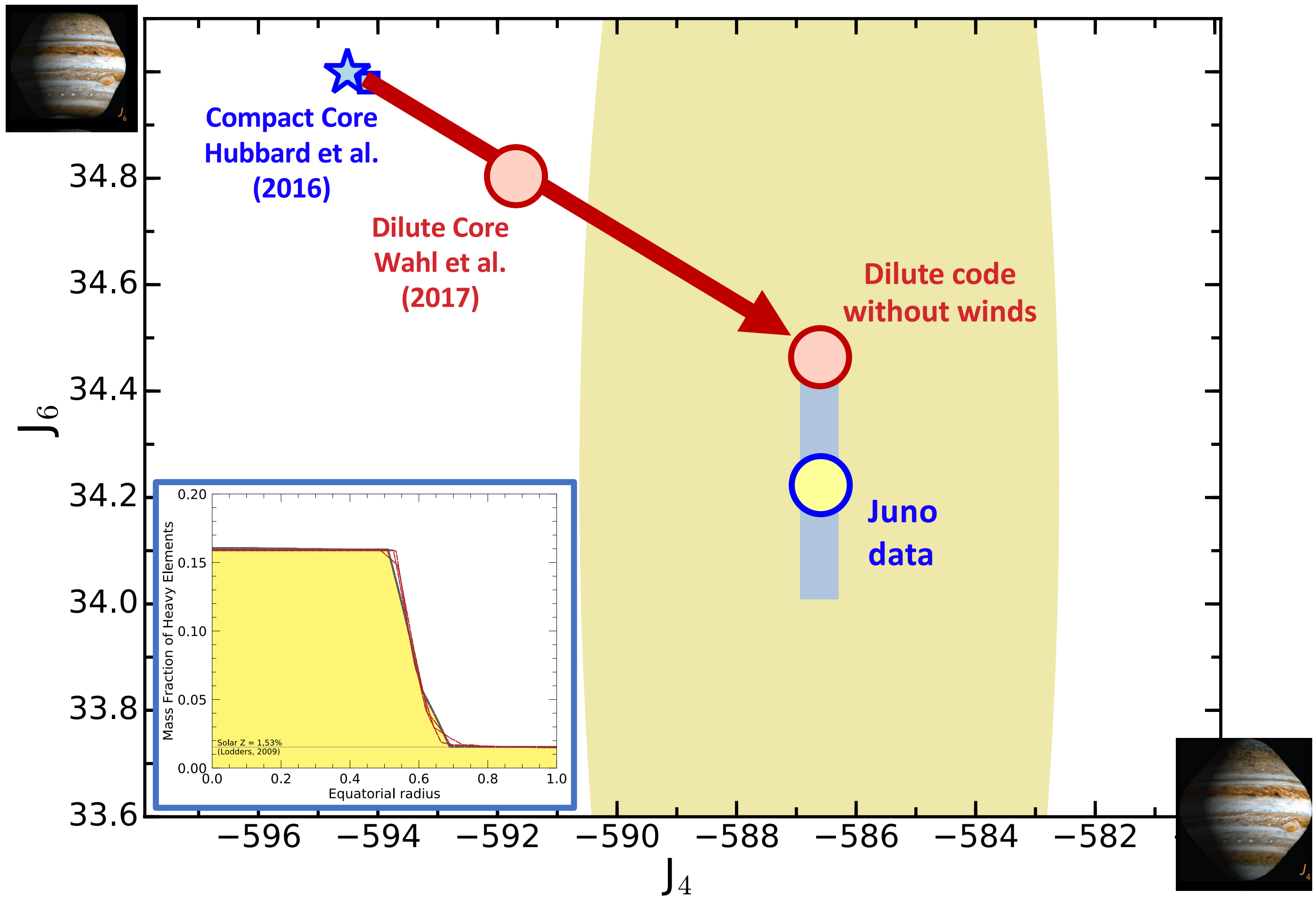
Compact Core Models (Hubbard, 2016) Do not Fit Juno's Gravity Measurements





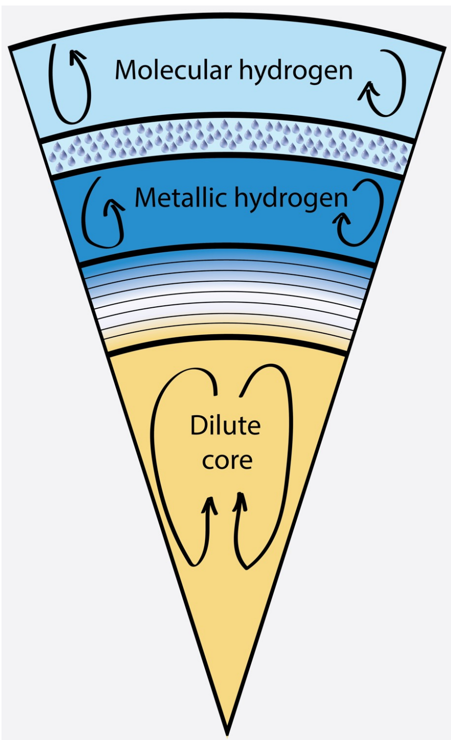
New Approach for Jupiter: Dilute Core
Simultaneous Optimization of Interior and Wind Models

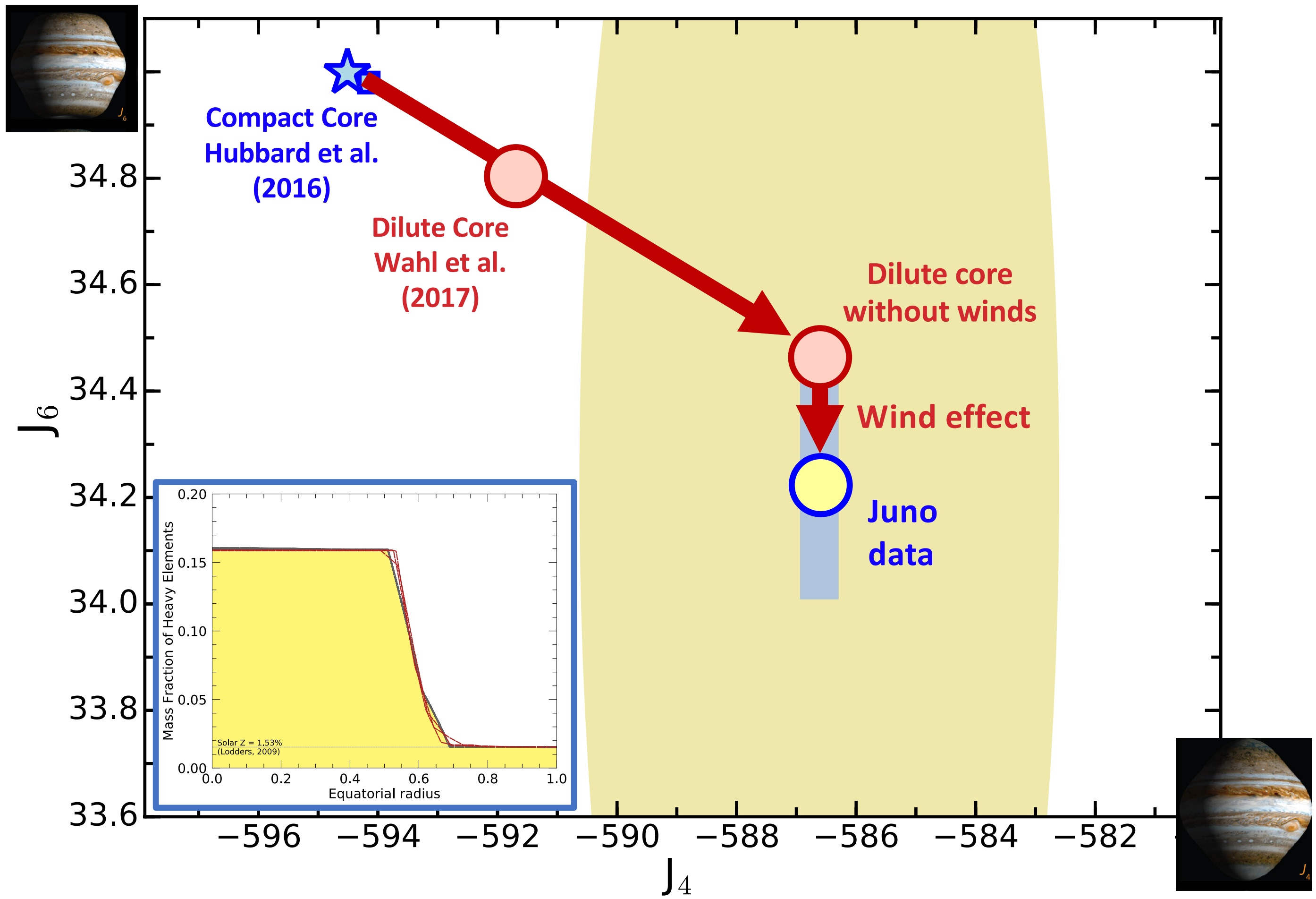




BM et al. Planet. Sci. J. (2022)

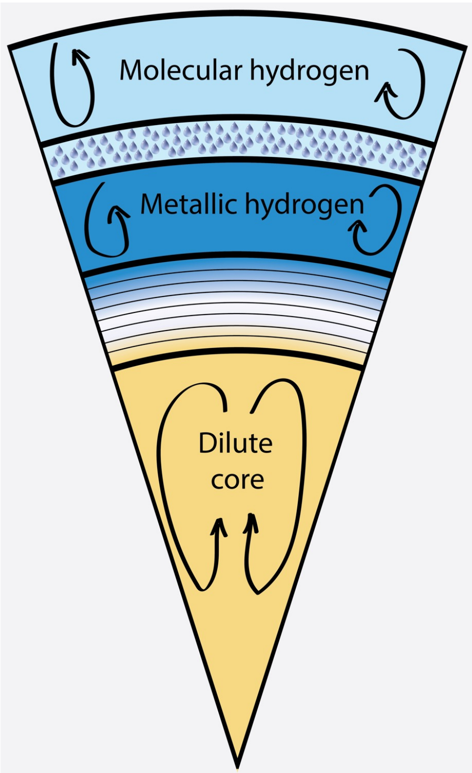
New Approach for Jupiter: Dilute Core
Simultaneous Optimization of Interior and Wind Models

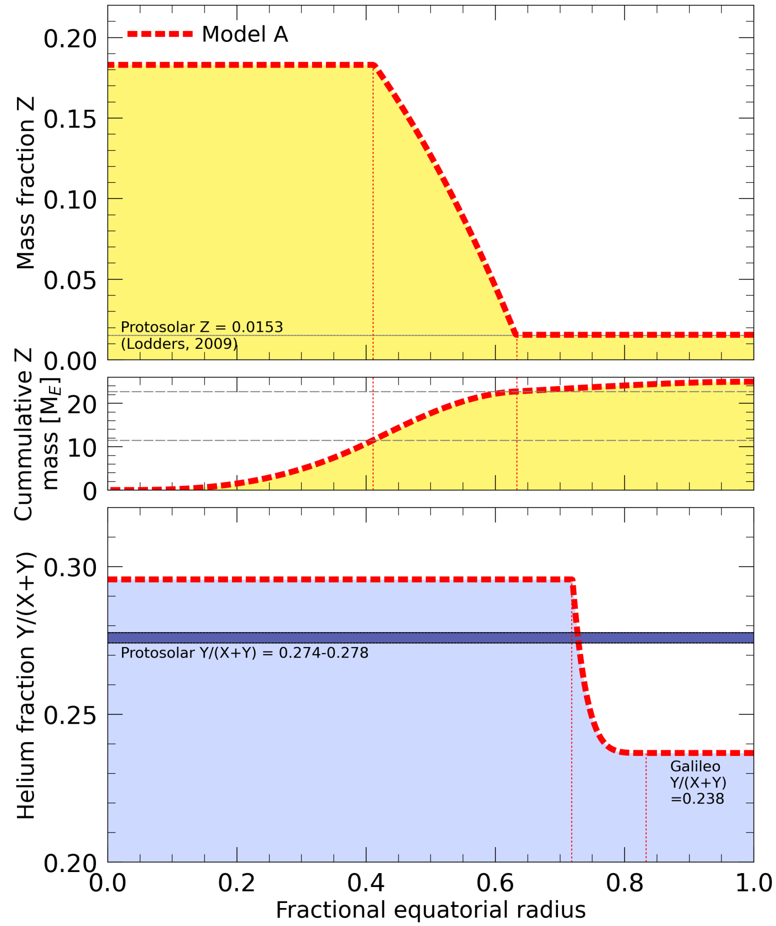




BM et al. Planet. Sci. J. (2022)

Five-Layer Model with Dilute Core for Jupiter's Interior





We can match all even and odd gravity coefficients under these assumptions.

BM et al, Planet. Sci. J. (2022)

Definition of tidal perturbation. Love number k_{22}

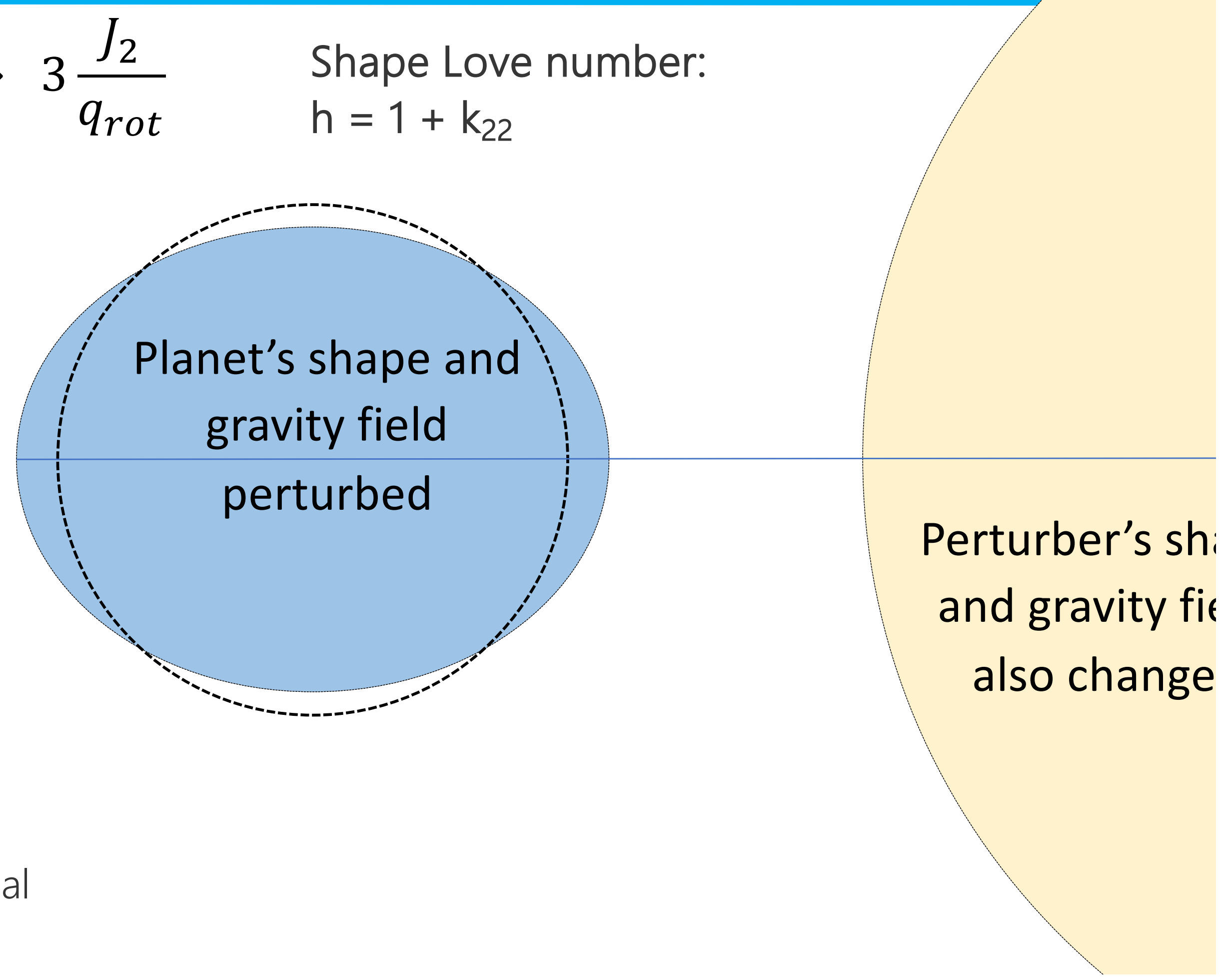
Perturbation of gravity

$$k_{22} = -\frac{16}{9}\frac{C_{22}}{q_{tide}} \longrightarrow 3\frac{J_2}{q_{rot}}$$

Shape Love number:
$h = 1 + k_{22}$

$$q_{tide} = -3\frac{M_{pert}}{M_{planet}}\frac{R^3_{planet}}{R^3_{orbit}}$$

$$q_{rot} = \frac{\omega^2 R^3_{planet}}{GM_{planet}}$$



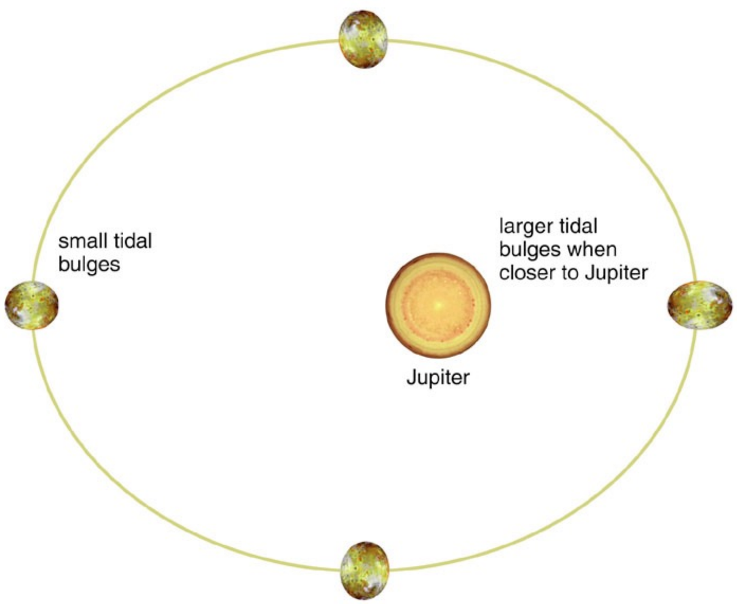
Static tides: Infinite time to establish hydrostatic equilibrium. Tidally locked case. Potential theory applies. Often a very good approximation. E.g Jupiter

Dynamic tides: Orbital frequency and rotation frequency differ. Perturber supplies energy. Tidal heating strong if orbits eccentric.

Two types of tidal interactions of giant planets

Planet interacts with orbiting satellites that may introduce dynamic tidal effects.

- Static tidal calculation k_{22}=0.590 (Wahl 2020)
- Juno mission k_{22}=0.565 ± 0.006
- Idini (2021): Coriolis acceleration $\Delta k_{22} = -4\%$



Exoplanet is tidally locked to host star which acts as tidal perturber. Rotation is thus slow.

- Planet changes shape. Apparent radius reduced by up to 4%.
- Planet's gravity field changes. (other planets)