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Pytesimal: A Python package for modelling small planetary bodies

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Summary

Planetesimals were small bodies that existed in the protoplanetary disk, some of which coalesced to form the planets, while others are sampled by the meteorite record. *TENSE ISSUE - not sure whether should be past or present? I hop around between them a bit...* Thermal processing recorded in meteorites can be linked to the thermal evolution of their parent planetesimals. This can inform us of the size and geometries of these parent bodies and how deep within them the meteorite material resided. *<- PHRASING SEEMS AWKWARD* Modelling the temperatures and cooling rates within planetesimals that existed 4.5 billion years ago is one of the key ways to understand the geological context of meteorites. The `Pytesimal` package focuses on the conductive cooling stage of planetesimal evolution, and provides a toolkit for modelling the temperature and cooling rate distribution inside meteorite parent bodies in 1D, with and without temperature-dependent material properties.

Statement of need

~~`Pytesimal` is a Python package for modelling the thermal evolution of planetesimals and other small planetary bodies.~~ *<- REPEATING MYSELF - but not sure whether to keep this line and instead get rid of last line of Summary section...* Meteorite parent body modelling is an active field in small-body planetary science. There are two broad categories of models: those focusing on the accretion and differentiation of planetesimals, and those investigating the later conductive cooling of parent bodies (Bryson et al., 2015; Elkins-Tanton et al., 2011; Haack et al., 1990; Murphy Quinlan et al., 2021; Nichols et al., 2016; Sahijpal, 2021). `Pytesimal` models the later conductive-cooling stage.

`Pytesimal` will enable groups to develop models of planetesimals and investigate the thermal history of meteorite parent bodies without having to rebuild the same basic architecture each time. `Pytesimal` provides a framework for modelling the conductive cooling of planetesimals, and is designed to be modular to allow future contributions and developments to be included. `Pytesimal` also includes plotting functionality to visualise the results of model runs, and a number of specialised tools designed to investigate pallasite meteorites specifically.

Method

The `Pytesimal` package focuses on the conductive cooling of differentiated planetesimals, with the ability to alter the model set-up to also investigate primitive bodies that have not segregated a core. The basic 1D set-up includes a conductively cooling discretised region which can include a low-diffusivity megaregolith layer, and an isothermal convecting core.

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The core can be removed to closer approximate primitive meteorite parent bodies, with a zero flux boundary condition applied across the centre to ensure symmetry (Figure 1).

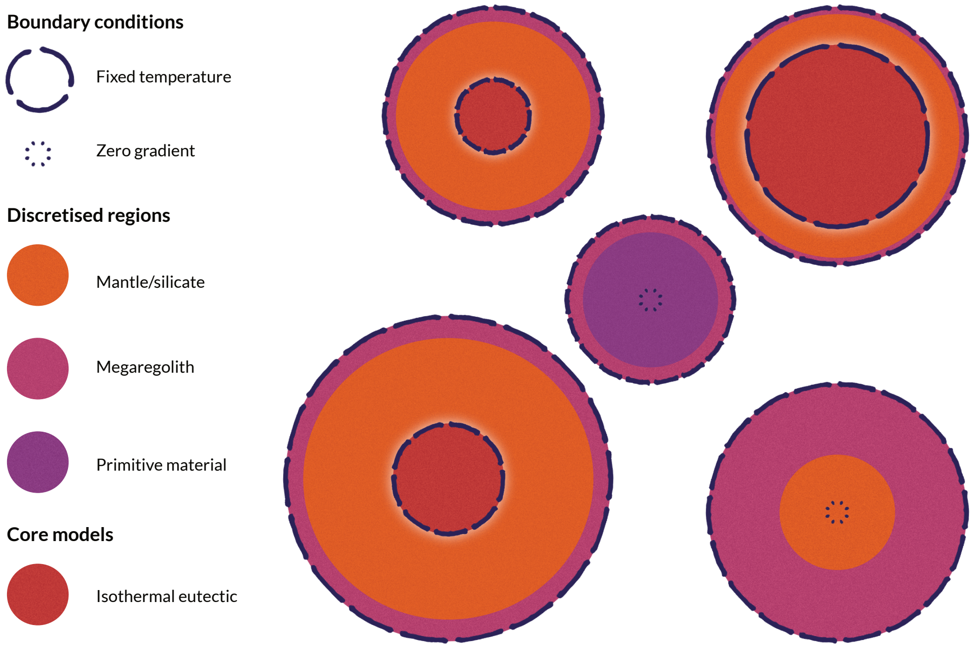

Figure 1: Cartoon sketch of model set-up. CHANGED COLOUR PROFILE TO CMYK

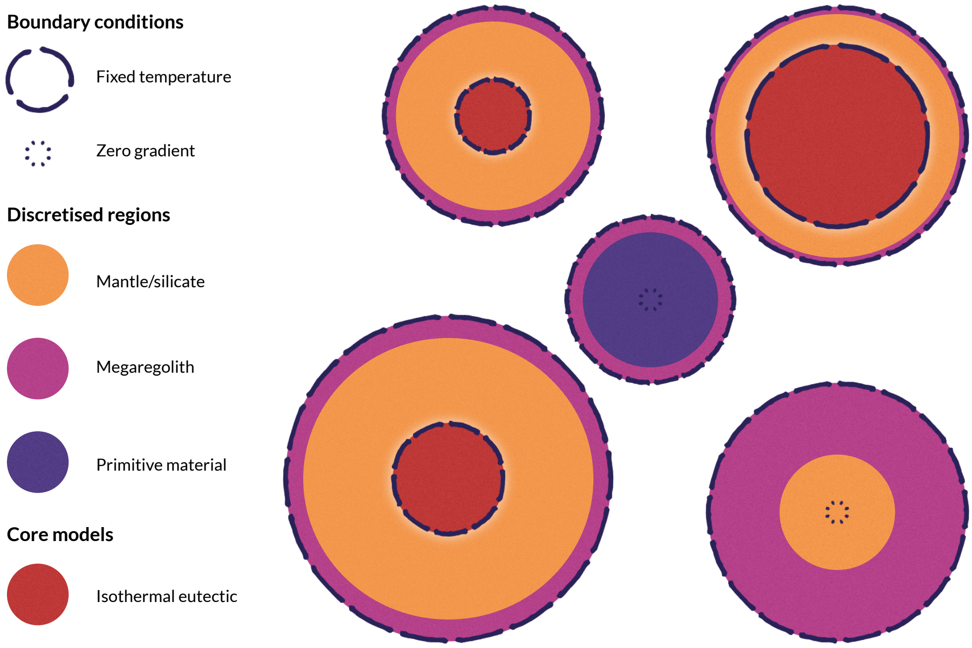

Figure 2: Cartoon sketch of model set-up. EDITED COLOUR PALETTE

The 1D conductive cooling of the discretised region is controlled by the heat equation:

$$\frac{\partial T}{\partial t}\rho C = \frac{1}{r^2}\frac{\partial}{\partial r}\left(kr^2\frac{\partial T}{\partial r}\right) = \overbrace{\frac{dk}{dT}\left(\frac{\partial T}{\partial r}\right)^2}^{\text{non-linear term}} + \underbrace{\frac{2k}{r}\frac{\partial T}{\partial r}}_{\text{geometric term}} + \overbrace{k\frac{\partial^2 T}{\partial r^2}}^{\text{linear term}}, \tag{1}$$

where T is the temperature, r is the radial value, t is time, and k, ρ and C are the conductivity, density and heat capacity respectively. `Pytesimal` provides the capability to use temperature-dependent conductivity, heat capacity and density, with functions suitable for an olivine mantle included. These T-dependent material properties of olivine (Figure 3) are based on experimental results and mineral physics theory from Fei (2013), Robie et al. (1982), Su et al. (2018), Suzuki (1975), Xu et al. (2004), with more information in Murphy Quinlan et al. (2021).

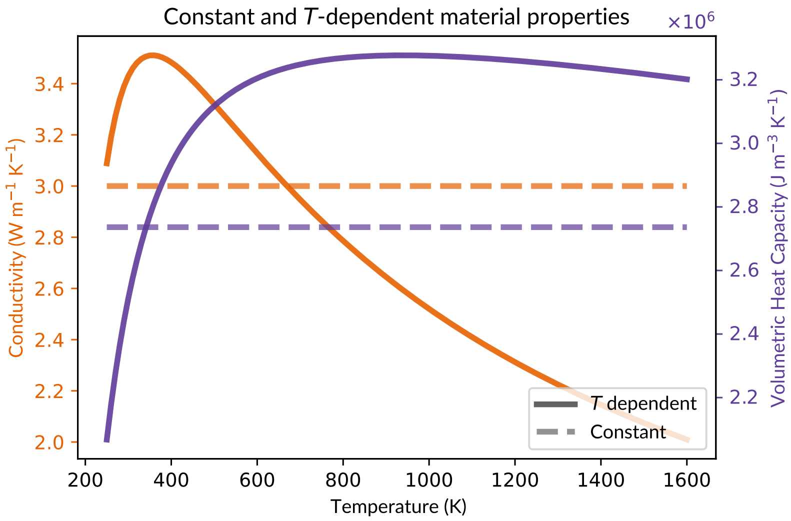

Figure 3: Conductivity (k) and volumetric heat capacity (ρC) in olivine.

The `numerical_methods` module uses the explicit Forward-Time Central-Space (FTCS) scheme which is conditionally stable and must satisfy Von Neumann stability criteria in 1D: $\frac{\kappa \delta t}{\delta r^2} \leq \frac{1}{2}$, where κ is the thermal diffusivity of the material, δt is the timestep of the numerical scheme, and δr is the radial step (Crank & Nicolson, 1947). `Pytesimal.numerical_methods` includes functions to calculate the diffusivity from k, ρ and C, and to check whether the chosen timestep will result in instabilities.

Boundary conditions for the top and bottom of the discretised region are passed into `numerical_methods.discretisation` as callable objects to allow for user-defined functions to be incorporated. Two different boundary conditions are currently provided, illustrated in Figure 3: a fixed temperature condition which can be applied to either the top or bottom boundary of the discretised region, and a zero flux boundary condition that can be applied at the bottom boundary when the core is removed.

The core interacts with the mantle through heat extracted across the core-mantle boundary over one timestep in the form of power (P, in Watts). The heat extracted in one timestep

(P_{CMB}) is calculated:

$$P_{\text{CMB}} = -A_{\text{c}} k_{\text{m}} \frac{\partial T}{\partial r}\bigg|_{r=r_{\text{c}}} \tag{2}$$

where A_{c} is the core surface area, r_{c} is the core radius, and k_{m} is the thermal conductivity at the base of the mantle or discretised region. From this, the core boundary temperature is then updated by ΔT:

$$\Delta T = -\frac{P_{\text{CMB}}}{\rho_{\text{c}} C_{\text{c}} V_{\text{c}}} \delta t \tag{3}$$

where ρ_{c} and C_{c} are the density and heat capacity of the core, and V_{c} is the volume of the core. Once the core reaches its freezing temperature, the temperature is held constant. Latent heat is extracted until the total latent heat associated with core crystallisation has been removed. This simple eutectic core model ignores inner core formation and treats the liquid and solid fraction as identical, but is implemented in a way that allows the `IsothermalEutecticCore` object to be replaced with a more complex core model where applicable.

`Pytesimal` also contains the functionality to quickly plot results, which allows for both on-the-go data visualisation and for saved results to be loaded and plotted at a later time (Figure 4). The `analysis` module can be used to calculate cooling rates, estimate the depth of pallasite meteorite genesis, and find the time when paleomagnetism could be recorded by these meteorite samples.

Examples of applications

~~An earlier version of~~ `Pytesimal` has been used in a scientific publication to demonstrate that the inclusion of temperature dependent thermal properties in place of constant values can result in different interpretations of the meteorite record, with pallasite meteorites used as an example (Murphy Quinlan et al., 2021). Figure 4 reproduces the results of Murphy Quinlan et al. (2021). The default values provided by `load_plot_save.make_default_param_file` are from Murphy Quinlan et al. (2021) and citations therein.

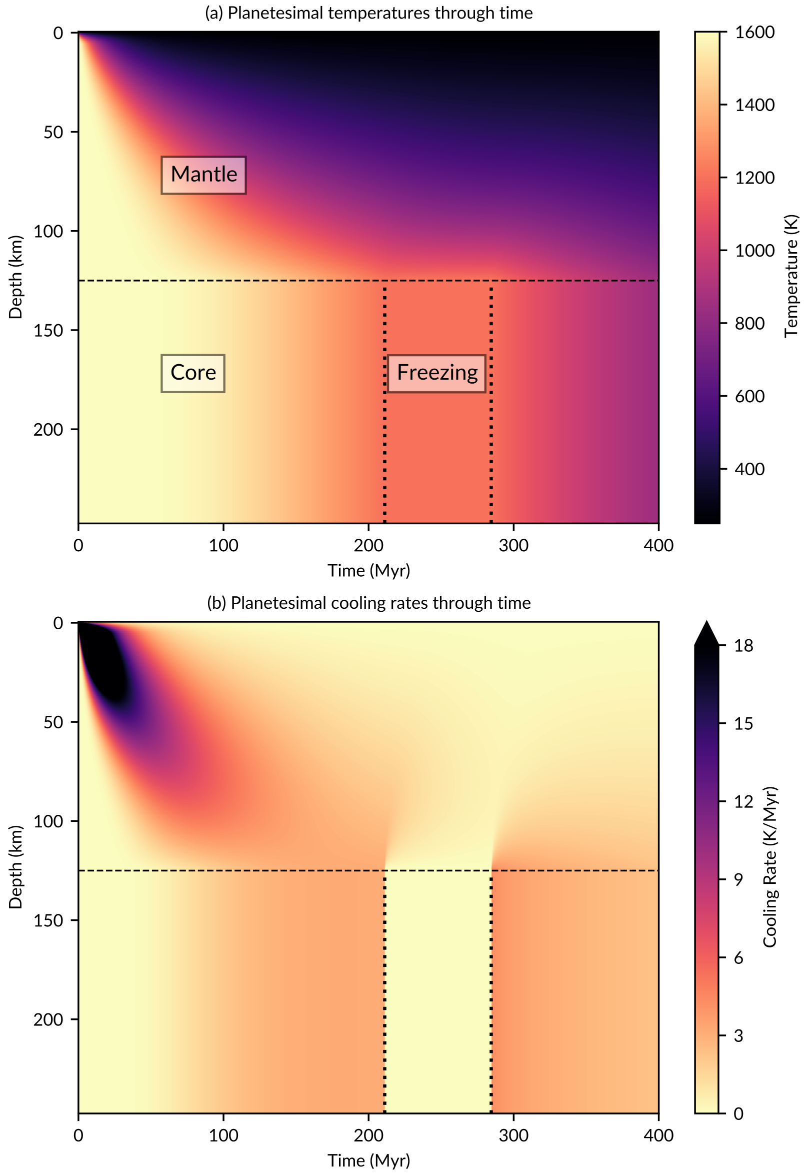

Figure 4: Temperatures and cooling rates in a 250 km radius planetesimal, using temperature dependent material properties. Annotations and lines to show the mantle, core and core crystallisation period are added later, outside of the `pytesimal.load_plot_save` functions.

Benefits of this package

1. `Pytesimal` only requires the commonly available Python packages `numpy` and `matplotlib`, with `Jupyter` useful for running the provided examples, but not essential.
2. Simple models can be set up and run in a single function call with an input parameter file, while more bespoke set ups only require a few extra lines of code.
3. `Pytesimal` is designed to be modular and extensible so that it can apply to a wide range of modelling requirements, to speed up development of meteorite parent body models.
4. Quick and simple visualisation of the results can be achieved with a single function call, and can be modified easily to produce publication-quality figures.

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