LARGE-SCALE NUMERICAL SIMULATIONS OF PLANETARY INTERIORS. A. C. Plesa¹, M. Maurice¹, S. Padovan¹, N. Tosi^{1,2}, D. Breuer¹. ¹German Aerospace Center (DLR), ²Technische Universität Berlin.

Introduction: The large amount of data returned from space missions and telescopes has helped to improve our understanding of the thermochemical evolution of terrestrial planets in our Solar System and beyond. However, the interior dynamics of terrestrial bodies is poorly constrained as direct constraints are lacking and laboratory experiments can only cover a limited parameter space often not representative of the deep interior. Over the past decades, large-scale numerical simulations of interior evolution have grown to become one of the most powerful approaches to model the temporal evolution of the mantle flow in the interior of terrestrial planets. Large improvements both in processor power and amount of available memory have made possible to tackle highly complex scenarios of planetary evolution by modeling vigorous convection at extreme Rayleigh numbers with highly variable viscosity and including chemical heterogeneities in a 3D spherical geometry.

Modeling the interior evolution of terrestrial planets: The thermochemical evolution of the mantle of terrestrial planets is modeled by solving the fundamental equations governing the conservation of mass, momentum and energy [1]. Convection driven by active chemical fields is modeled with the particle in cell method (PIC) [e.g., 2, 3, 4]. This method employs Lagrangian tracers that carry various chemical species, and has the advantage over classical grid-based methods of being essentially free of numerical diffusion. It also provides the advection of an arbitrary large number of different compositional fields with less computational effort.

We use the fluid flow solver Gaia, which is written in library-independent C++ (except MPI that can be disabled), making it easy to port on all type of systems. Gaia uses the finite-volume method to discretize the governing equations on arbitrary grids in various geometries as long as they are Voronoi grids [5, 6].

An efficient domain decomposition of a given computational mesh results into *n* equal volumes, with each volume being mapped to a computational core. While for 3D Cartesian box grids, due to their regular nature, an optimal domain decomposition can be easily achieved, the problem becomes highly complex when 3D spherical shells are involved. In Gaia we use the so-called Thomson-points to laterally decompose the sphere by distributing points, all assumed with equivalent potential energy, on the surface of the sphere and minimizing the global potential field energy. The closest Thomson-point defines the domain of every grid cell [7, 8].

We tested the performance of our code on the Hazel Hen system of HLRS using up to 54×10^3 computational cores (dual socket Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.5 GHz having two sockets per node with 12 cores each). To this end we have performed numerical simulations using a 3D Cartesian box regular grid with 55 million computational points (275 million unknowns) and a 3D spherical shell fully irregular grid with 12 million computational points (60 million unknowns) and additional 240 million tracers. The strong scaling achieved with the two setups is shown in Fig. 1a. For the 3D Cartesian box grid we used up to 54 x 10^3 cores, while the 3D spherical shell simulation has been performed with up to 13×10^3 cores. The domain decomposition for the 3D spherical shell grid used 2 radial and 4352 lateral slices (4352 being the largest amount of available Thomson-points). Fig. 1b-d shows a typical domain decomposition for various meshes.



Fig. 1: a) Gaia code performance with up to 54×10^3 computational cores using a 3D Cartesian box grid with 55 million cells (green line) and a fully irregular spherical shell grid with 12 million cells (red line); Domain decomposition b) on 32 processors for a Cartesian box grid containing 1 million cells; c) on 16 processors for a partial sphere grid containing 1 million cells; d) on 255 processors for a fully irregular 3D spherical shell grid using a finer resolution towards the surface and a total of 8 million computational cells.

Application to mantle convection: Magma ocean crystallization and onset of solid-state convection. In the early stages of planetary evolution, the amount of heat available from accretion and core formation processes as well as from the decay of short-lived radioactive nuclides like ²⁶Al and ⁶⁰Fe is thought to have caused multiple episodes of extensive melting of the silicate mantle leading to local or even global magma oceans [9].

A better understanding of the solidification of a liquid magma ocean is essential for constraining the subsequent planetary evolution, but so far the crystallization process is poorly understood. For example, various studies predict a crystallization sequence of the Martian magma ocean that is difficult to reconcile with the subsequent thermochemical evolution and longlived volcanic activity of the planet. Previous studies of magma ocean solidification have assumed an undisturbed crystallization process leading to a gravitationally unstable layering of the mantle that may cause an overturn [e.g., 10]. However, the density distribution attained during the crystallization process can be strongly influenced by the onset of solid-state convection prior to complete solidification. In a recent study, we investigated the mixing behavior in the Martian mantle during the crystallization of a global magma ocean and found that compositional heterogeneities established during the solidification can be partly or even entirely erased [11].

Thermochemical evolution of Mercury. We have applied our code to model the thermochemical evolution of Mercury and to predict crustal production and duration of magmatic activity that can be compared to the observations of the MESSENGER mission. This comparison led to inferences about the bulk abundance of radiogenic elements in the interior of the planet and the duration of volcanic activity [12]. The latter is compatible with the dating of the youngest large volcanic provinces [13]. Moreover, including the effects of large impact basins on the thermal evolution, we showed that it is possible to connect the local datasets relative to the large impact basins on the planet with its global thermal evolution, possibly providing a pathway to explain some of the geochemical anomalies associated with the interior of large impact basins [14].

Present-day surface heat flow of Mars. We have shown that the spatial variations of crustal thickness and the pressure dependence of the viscosity are responsible for the spatial distribution of surface heat flow and most likely affect the formation and location of mantle plumes [15]. Mantle plumes are directly related to partial melt production in the mantle and are thought to be responsible for the youngest volcanic activity in Tharsis and Elysium volcanic provinces. Nevertheless, our simulations predict that mantle plumes are unlikely to affect the upcoming surface heat flow measurements that will be performed by the InSight mission [16] and the heat flow values at the landing site in the Elysium Planitia region would be representative of the present-day average surface heat flow of Mars [15]. Moreover, using a number of constraints from the Martian geological record, (e.g., the evolution of the elastic lithosphere thickness, longlived partial melt production in the mantle and geodetical estimates), along with a large set of numerical simulations, we can identify a best fit model of the Martian interior, which can be tested and validated with the upcoming seismic and heat flow measurements of InSight.

Conclusions and Outlook: Numerical simulations of interior dynamics can be applied to investigate the thermal evolution of a terrestrial body from the earliest stages up to the present day. Such models can be employed to interpret upcoming measurements in a global context and to link surface observations to the interior evolution. Moreover, with the increase of computational resources, the large amount of data produced by numerical thermal evolution models can be combined with machine learning algorithms and deep neural networks to identify key parameters that control the evolution of terrestrial bodies. This combination is a promising approach that has only started to be included within the scope of linking input parameters necessary to run thermal evolution models with available planetary mission data and observations.

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