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A particle-in-cell method for studying double-diffusive convection in the liquid layers of planetary interiors

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ABSTRACT

Many planetary bodies contain internal liquid layers in their metallic cores or as buried water oceans. Convection in these layers is usually driven by buoyancy sources of thermal or compositional origin, with very different molecular diffusivities. Such conditions can potentially trigger double-diffusive instabilities and fundamentally affect the convective features. In numerical models, the weak diffusivity of the compositional field requires the use of a semi-Lagrangian description to produce minimal numerical diffusion. We implemented a "particle-in-cell" (PIC) method into a pre-existing geodynamo code in 3D spherical geometry to describe the compositional field properly. We developed several numerical strategies to solve various problems inherent to the implementation of a PIC method for convection in spherical geometry and coded a hybrid scheme suitable for massively parallel platforms. We tested our new code on two benchmark cases which validate its applicability to the study of double-diffusive convection in the internal liquid layers of planets. As a first application, we study a case of non-magnetic double-diffusive convection at infinite Lewis number. Major differences emerge both in the compositional field and the convective pattern when the compositional diffusivity is neglected.

1. Introduction

Numerous planetary bodies contain internal liquid layers in the form of either partially liquid iron core, buried water oceans [26,28,11], post-accretion primitive magma oceans [30] or metallic hydrogen in giant gas planets [22]. The presence of convective currents within such layers can generate magnetic fields by dynamo action in planetary cores like those of the Earth, Mercury and Ganymede [7,13,27], affect the geology of the surface ice of icy satellites such as Ganymede, Europa and Enceladus [39,45,44], and influence the dynamics of a crystallizing magma ocean in the young Earth [30]. Convection in these layers is usually driven by the combination of two sources of buoyancy: a thermal source directly related to the planet's secular cooling, the release of latent heat and possibly the heat generated by radioactive decay, and a compositional source due to some process of crystallization or fusion, for example the growth of a solid inner core which releases light elements into the liquid outer core [7], or the melting/freezing of an ice layer which locally enriches or depletes the adjacent

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water ocean in salts [55]. Other potential compositional buoyancy sources may also include precipitation of magnesium or crystallization of silicon dioxide at the Earth's core mantle boundary [40,56].

The molecular diffusivities of the thermal and compositional fields typically differ by several orders of magnitude: the Lewis number (ratio of the thermal to the compositional molecular diffusivity) is at least 100 in oceans [47] and 1000 in the Earth's outer core [7] which can potentially generate "double-diffusive" instabilities [53] leading to significant differences in the convective dynamics compared to pure thermal or compositional convection, respectively.

The classical approach proposed by Braginsky and Roberts [7] and the same year by Lister and Buffett [33] has been widely adopted since [29,16,4,46,14,1,37] and consists of combining both sources of buoyancy into a single component named codensity, under the assumption that the mixing action of the unresolved sub-grid-scale turbulence would lead to comparable effective diffusivities. Codensity is a very convenient approach since it is easy to implement in codes of geodynamo and does not increase the computational demand, but it remains limited and simplistic. First, in liquid cores and oceans, the thermal and chemical boundary conditions usually differ and should be included as distinct conditions for the two fields. In addition, these are coupled through the melting/freezing process at the interface. This cannot be properly described by the codensity approach and requires the fields to be treated separately. Second, due to the complexities of core turbulence, codensity is presumably a rough approximation even in the case of highly turbulent regimes since turbulent mixing in the core is probably anisotropic [7]. The use of codensity may be even more problematic inside stratified layers, the existence of which has been evoked for some planetary cores [35,14] and even for the Earth [24]. In such context, it is likely that turbulence will be much less efficient if not absent and that the mixing of properties will rather be performed by molecular diffusion [7]. For a more general and rigorous modeling, one should therefore solve two distinct transport equations for temperature and composition using two different diffusivities, or even neglecting the compositional diffusivity.

This "double-diffusivity" scenario has recently received much attention by a few authors [8,35,51,50] but these studies were conducted only up to a moderate Lewis number of 10 for technical reasons. Indeed, on the one hand, solving the advection-diffusion equation with a small diffusivity makes it compulsory to use very high resolutions in order to avoid numerical oscillations (the grid Peclet number $Pe = u\Delta x/\kappa$ should be less than about 1 everywhere in the grid, u being the local velocity, Δx the local grid spacing and κ the diffusivity). On the other hand, solving the hyperbolic equation (by neglecting the diffusive term) in Eulerian methods to explore the infinite Lewis number case leads to problems related to numerical diffusion [38]. An alternative solution is to opt for diffusion-free semi-Lagrangian representations such as *"particle-in-cell"* (PIC) methods. PIC methods (also referred to as *"marker-in-cell"* or *"tracer"* methods) have been formalized in the late 1950s [18] and developed since into a series of variants ranging from mostly Eulerian to quasi fully Lagrangian methods to address diverse physical problems in hydrodynamics [6,43], plasma physics [10,5,25,21,52], astrophysics [42] and meteorology [31], mostly in 2D and 3D Cartesian geometries. In Earth and planetary sciences, PIC methods have been successfully employed for solid-state mantle convection [49] but they have never been used for convection in planetary cores or liquid oceans, to our knowledge. In this work, we implemented a PIC method into a pre-existing geodynamo code to extend its range of applications to the study of double-diffusive convection in the liquid layers of planetary interiors at infinite Lewis number. The fundamentals of the method remain similar to those of previous studies, but extra technical difficulties arise, mostly due to its implementation in spherical geometry as well as the properties of the flow influenced by rotation and magnetic field.

In section 2, we describe in detail the principle of this PIC method and propose a few approaches to various problems inherent to the spherical geometry. The results of the benchmark tests we performed to validate this new code are shown and analyzed in section 3. We then address critical questions regarding the adequate number of tracers and also discuss the code's performance and its adaptation to High Performance Computing (HPC) architectures. In the final section, we show a first application of our code by running two simulations of non-magnetic convection at infinite Lewis number. The properties of the flow are compared to that of an analogous case at a moderate Lewis number.

2. Numerical method

2.1. Principal equations

The modeling of core dynamics is usually performed by solving the equations for the conservation of mass, energy, momentum and magnetic induction in a rotating and electrically conducting spherical shell of inner and outer radii r_i and r_o, respectively, under the Boussinesq approximation. The modeling of oceanic convection in icy satellites can be performed in a similar way by ignoring any magnetic effect. The fluid considered is a mixture of a dominant component (iron in a metallic core) and a light constituent, whose compositional mass fraction is denoted by C and varies from $C = 0$ (pure iron) to $C = 1$ (pure light elements). In this context, the density can be modeled as a function of both temperature, T, and compositional mass fraction, C:

$$\rho = \rho_0[1 - \alpha(T - T_0) - \beta(C - C_0)], \tag{1}$$

where T_0, C_0 and ρ_0 are the reference temperature, composition and density, respectively. α is the thermal expansivity and β its analogous compositional coefficient. Two distinct transport equations must thus be solved and are written, in their dimensional form: