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Progress towards physics-based space weather forecasting with exascale computing

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ABSTRACT

Space weather is a rapidly growing field of science which studies processes occurring in the area of space between the Sun and the Earth. The development of space weather forecasting capabilities is a task of great societal relevance: space weather effects may damage a number of technological assets, among which power and communication lines, transformers, pipelines and the telecommunication infrastructure. Exascale computing is a fundamental ingredient for space weather forecasting tools based on physical, rather than statistical, models. We describe here our recent progresses towards a physics-based space weather forecasting tool with exascale computing. We select the semi-implicit, Particle In Cell, Implicit Moment Method implemented in the parallel, object-oriented, C++ iPic3D code as a promising starting point. We analyze the structure and the performances of the current version of the iPic3D code. We describe three algorithmic developments, the fully implicit method, the Multi-Level Multi-Domain method, and the fluid-kinetic method, which can help addressing the multiple spatial and temporal scales present in space weather simulations. We then examine, in a co-design approach, which requirements – vectorization, extreme parallelism and reduced communication – an application has to satisfy to fully exploit architectures such as GPUs and Xeon Phi's. We address how to modify the iPic3D code to better satisfy these requirements. We then describe how to port the iPic3D code to the DEEP architecture currently under construction. The FP7 project DEEP (www.deep-project.eu) aims at building an exascale-ready machine composed of a cluster of Xeon nodes and of a collection of Xeon Phi coprocessors, used as boosters. The aim of the DEEP project is to enable exascale performance for codes, such as iPic3D, composed of parts which exhibit different potential for extreme scalability. Finally, we provide examples of simulations of space weather processes done with the current version of the iPic3D code.

1. Introduction

Space weather [1–4] is the fast-growing area of science that focuses on the conditions in the space amidst the Sun, the Earth and the other planets of our solar system. The Sun is an extremely dynamic source of energy. Besides the electromagnetic radiation (including of course light) that makes life possible, the Sun is a giant dynamo that produces a strongly magnetized plasma. The plasma flows away from the Sun at supersonic speeds, arriving at the Earth with velocities ranging from about 200 to 800 km/s. This wind is very dynamic and varies greatly. Just like Earth winds, it also carries storms. The most powerful space storms are generated irregularly in singular events of mass and energy released by the Sun, called coronal mass ejections. The intensity and frequency of these storms oscillates over the course of a solar cycle, with a period of about 11 years. Peak activity is called solar maximum (solar maxima occurred in 2000 and in 2013) and is separated by periods of very low activity at solar minimum (2008–2009). Solar activity also changes on much longer scales. Generations of scientists have monitored the solar activity since the 17th century. The solar cycles of the space age, following the first space trip of Yuri Gagarin, have happened to be particularly active. However, a period of prolonged quietness lasting several decades happened in the end of the 17th century. It is called the Maunder minimum and corresponds to a period of exceptionally cold winters and insufficient crop production in Europe. Since this period, at least one exceedingly strong

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event, the Carrington event, happened in 1859, causing severe telegraph disruptions back in those early industrial revolution days. A similar event now would wreak havoc on our space technology and on our ground infrastructure, such as, as examples, power and communication lines, transformers, pipelines and telecommunication infrastructure. A Carrington-sized event now could not only render multiple satellites permanently inoperative but could damage beyond repair the largest transformers on the highest voltage long distance power lines. These transformers and satellites would require several months to replace. One can clearly see that a blackout lasting months would greatly disrupt the economy and social tranquility. One has also to take into account that past blackouts caused by space weather events involved especially the northeast of the American continent, because of the geographical location of the magnetic north pole. The area includes some of the world's most active financial trading and data centers. This brief summary explains why space weather has become a key area of scientific computing. Predicting space weather is a top priority to defend key societal infrastructures and to expand the human presence in space. All major industrialized and developing countries are developing a space weather forecasting capability, with both military and civil agencies contributing to the effort at national and international levels. All these activities center on one key ingredient: the reliance on physics-based high performance computing codes that can follow a space storms from its origin on the Sun to its consequences at Earth. These models are very complex and must include many processes and aspects, including the sheer size of the vastness of the space involved and the great variety of conditions encountered from the hot solar corona to the cold depths of deep space. Density and temperature change over many orders of magnitude. In space, matter is in the form of plasma. Atoms are ionized and electrons are freed from their bond to the nuclei of atoms. Electrons, being much lighter than the nuclei (for hydrogen the mass ratio between nuclei and electrons is 1836), respond on much smaller scales. The physics-based description of space (see, for example, [5] for an alternative, statistical description of the solar wind propagation from the Sun to Earth) requires handling multiple scales in space and time and multiple physical processes. Dealing with multi-scale and multi-physics systems is the key challenge in modern high performance computing (HPC), common to many other engineering and science applications. Even the largest supercomputers can only cover a limited range of scales and physics, posing a great challenge to co-design: how to design new computer architectures and new algorithms so that the gaps are filled and a complete answer can be found for multi-scale and multi-physics challenges.

Here we detail the approach followed in our co-design effort for HPC applied to space weather modeling. The paper is organized as follows. First, we describe our target application: kinetic modelling of space weather, using the Particle In Cell (PIC) approach. Section 2 describes the basics of the Particle In Cell method, i.e. space discretization of field values at grid points and representation of ions and electrons as computational particles moving in the continuum. In Section 2.1 we describe an implicit temporal discretization of the equations for the temporal evolution of fields and particles. The implicit discretization has the advantage of making PIC simulations computationally cheaper with respect to explicit formulations. It relaxes the constraints in terms of spatial and temporal resolution for the stability of the simulation. It also has the algorithmic disadvantage of coupling the equations for field and particle time advancement: to advance in time the electric and magnetic fields, we now need information on particle position and velocity at the future time step, and vice versa. We describe in Section 2.3 the Implicit Moment Method (IMM), a method to remove the coupling between the field and particle sets of equations. The IMM has been implemented in the parallel, object-oriented, C++ code iPic3D [6], described in Section 2.4. In Section 2.5, the iPic3D code is broken into four logical blocks. The relative weight of these blocks in terms of execution time and communication requirements is investigated on different clusters and with different problem sizes. The Scalasca performance analysis tool is used in the investigation. Section 3 and Section 4 are the core of this paper. There, we analyze the progress that we recently achieved and that will enable an effective and efficient use of PIC methods for space weather forecasting. The progress reported follows two intertwined lines: development of new algorithms and identification of co-design issues.

On the algorithmic line (Section 3), we report model development designed to handle multiple spatial and temporal scales. The temporal discretization has been improved to reach exact energy conservation (Section 3.1), a crucial aspect to guarantee that simulations faithfully reproduce reality. The discretization capabilities have been expanded: it is now possible to use multiple levels of spatial and temporal resolution to describe different levels of physical refinement in different regions. The resulting method, the Multi-Level Multi-Domain method, is described in Section 3.2. Finally, a new hybrid approach that extends the ability to include multiple physical descriptions based on kinetic or fluid methods has been developed (Section 3.3)

Co-design aims at establishing continuous and effective feedback between the code development and machine design stages. On one side, algorithms must be deviced as to exploit at best the characteristics of exascale-oriented machines: parallelization must be increased, communication reduced. On the other end, the requirements coming from cutting-edge scientific fields, such as space weather, have to be considered in the design of next generation HPC machines. In Section 4 we describe how the issues of vectorization, communication and parallelization (Section 4.1) apply to the code iPic3D and to fully kinetic simulations of space weather, and in which directions we plan on developing iPic3D to better comply with the programming models required to exploit at best GPU/ Xeon Phi architectures (Section 4.2). We also report our experience (as of 2014) within the DEEP project, which aims at building an exa-scale enabling machine constituted by a traditional cluster of Xeon nodes plus a collection of Xeon Phi coprocessors (Section 4.3). Finally, in Section 5, we conclude with some examples of the capabilities of the IMM and of the iPic3D code of simulating space weather relevant processes: transfer of magnetic energy to particles in simulations of null points dynamics in 3D (Section 5.1) and solar wind/ magnetosphere interaction (Section 5.2).

2. Target application: kinetic modeling of space weather

The fundamental agents of a space weather simulation are the electric and magnetic fields that permeate space and the particles moving through them.

The field evolution is described by the equations of Maxwell

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$
$$\nabla \times \mathbf{B} = \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J}, \tag{1}$$

for the electric field $\mathbf{E}$ and the magnetic field $\mathbf{B}$, with ϵ_0 and μ_0 the permittivity and permeability of free space respectively. The particle evolution is described by the equations of Newton,

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p,$$
$$\frac{d\mathbf{v}_p}{dt} = \frac{q_s}{m_s}(\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p), \tag{2}$$

for the position $\mathbf{x}_p$ and velocity $\mathbf{v}_p$ of each particle labelled by p. Particles are organized in species (e.g. electrons, ions) labelled

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