Macro-Micro Interlocked Simulator[†]

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Abstract Simulation Science is now standing on a turning point. After the appearance of the Earth Simulator, HEC is struggling with several severe difficulties due to the physical limit of LSI technologies and the so-called latency problem. In this paper I would like to propose one clever way to overcome these difficulties from the simulation algorithm viewpoint. Nature and artificial products are usually organized with several nearly autonomously working internal systems (organizations, or layers). The Earth Simulator has gifted us with a really useful scientific tool that can deal with the entire evolution of one internal system with a sufficient soundness. In order to make a leap jump of Simulation Science, therefore, it is desired to design an innovative simulator that enables us to deal with simultaneously and as consistently as possible a real system that evolves cooperatively with several internal autonomous systems. Three years experience of the Earth Simulator Project has stimulated to come up with one innovative simulation algorithm to get rid of the technological barrier standing in front of us, which I would like to call "Macro-Micro Interlocked Algorithm", or "Macro-Micro Multiplying Algorithm", and present a couple of such examples to validate the proposed algorithm. The first example is an aurora-arc formation as a result of the mutual interaction between the macroscopic magnetosphere-ionosphere system and the microscopic field-aligned electron and ion system. The second example is the local heavy rain fall resulting from the interaction between the global climate evolution and the microscopic raindrop growth process. Based on this innovative feasible algorithm, I came up with a Macro-Micro Multiplying Simulator.

Keywords: Earth Simulator, Simulation Science, Macro-Micro Interlocked (MMI) Algorithm, MMI Simulator

1. Introduction

In the 60 years elapse of Computer Simulation since the birth of ENIAC, three epoch-making computer technological innovations are to be noted. The first one is the invention of the semi-conductor in 1948. Undoubtedly, it was the semi-conductor invention that has brought today's prosperity of simulation science. The second one, and the most simulation oriented innovation, is the Seymour Cray's vector architecture in 1976. The third one is the parallel architecture that connects processors (or processor nodes) via an interconnection network. The advantage of this parallel architecture is to increase the theoretical peak flops by summing up the peak flops of all connected processors.

The Earth Simulator (ES) is the successful product of taking advantage of the vector and parallel architectures. Let me pick up a couple of reasons for the great success of ES among many. The vector architecture was employed and one-stage interconnection network system could succeed in drastically reducing the so-called latency overhead because of the smallness of the parallelism (640 processor nodes).

2. What the Earth Simulator has given us

The goodness of the ES is certainly its excellence of sustained performance for almost any scientific problems [1]. Besides, I would like to point out a much more important impact the Earth Simulator has brought us upon science. In our present Western science our attention has been paid primarily to revealing the past history of how the present Universe has been created and governed, and consequently, we have discovered almost all fundamental (elementary) laws that are governing the activity of the current universe, except the evolutionary equations of life. Although we have devoted all our efforts to developing mathematical tools to know and formulate the mechanism of revealed elementary laws, we have unfortunately left behind us our enthusiasm of

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invention of the tool to know the future evolution. This is because the future is not that simple and is a complex manifestation resulting from closely and highly tangled numerous elementary laws.

In the meantime, computer simulation was born to challenge to this complex problem towards the end of the World War II. In this sense, it would not be any exaggeration to say that simulation is the ultimate tool to science.

I would say that it is the ES that has awakened us to realize "Time has come". The ES has indeed recognized us that the future world has entered into the realm of science. More specifically, the future becomes the world of "Science Reality" which is so far treated as Science Fiction. This implies that future evolution of nature such as prediction of climate change and prediction of natural disasters are now in our hand, and also that new materials and products can be developed without making numerous, high-cost, time-consuming experimental tests as we usually do so[2].

Since the products obtained by the ES to demonstrate the above-mentioned statement are given elsewhere, I hope, interested readers should reach there (Annual Reports and the Journal of the Earth Simulator published by the Earth Simulator Center [3, 4]).

3. Beyond the Earth Simulator

The real purpose of this paper is not confined within the territory of the ES. Our precious time should be spent for our global design of the 21st Century Simulation Science, and, more, the 21st Century Science itself.

As everyone is aware of it, we are now facing two essential computer technological problems lying in front of us. The first one is the fact that the LSI is approaching to the physical limit of its size (~10nanometer) as a semiconductor element. This indicates that an avoidable physical limit is around the corner, no matter how enthusiastic we are and that there is no way to sky-high enhancement of chip performance as we used to. The smart way of getting out of this difficulty was to connect the same processor in parallel as many as we want, so that the face value of the performance can be increased linearly with the increase of the number of connected processors. However, as is well known, because of the increase of the communication overhead in square of the number of processors, sustained performance is drastically reduced, particularly when the parallelism exceeds ten thousands (note that the ES connects 640 processor nodes). This becomes more serious when the performance of a processor is more enhanced, like one Telaflops.

Unless we develop a really innovative communication technology, it would be a formidable task. Then, we have to patiently wait until such an innovation would come up some day and until that day we are supposed to do our gradual simulation research by using the existing computers day by day. Certainly such steady work is necessary and important to weed and plow the field, once it turns out to be able to grow crops. As far as we rely on the existing machines, however, only crops of the similar type and quality can be produced. No innovative and unpredictable crops would not be discovered.

Now turn our eyes to the workings of nature. We can find that in any system, all spatial and temporal scales are not fully occupied by energy or information. Energy and information are always concentrated in several discrete spatial and temporal scale domains in a system. This is because if all spatial and temporal scale domains are fully occupied with information or energy, then the system must be inactive and dead, thus, uninteresting. That nature is active and meaningful is equivalent to saying that nature is hierarchical, stratified, or, multiply organized. This is also the case for any goods or products created by humans. Information and energy are usually discretely localized in spatial and temporal scale domains of any system, say, microscopic and macroscopic.

Recall here that the ES has made it possible to deal with an entire system. To be precise, the ES can make it possible to deal with an entire system of only one internal system (organization) governed by the same physical law. Therefore, the other organizations adjacent to this organization must be plugged in as parameters and environmental conditions. Usually all related organizations (layers) are closely related to mutual evolution, hence, we call a system. Therefore, future predictions made by the ES, for example, global warming, include scientific uncertainties. There exists relatively large arbitrariness in the choice of parameters and environmental conditions. This parameterization procedure is unavoidable because even the ES is too small to deal simultaneously and self-consistently with two mutually cooperating adjacent organizations together. This is because to deal with two cooperating organizations simultaneously and self-consistently requires connection of some hundred millions of Earth Simulator scale computers, namely, an ultra-massively connected simulators system.

Could you believe that such a giant computer system can be realized in 20 years from now on? The answer is absolutely negative.

In light of the fact that the ES has enabled us to deal with an entire system of one organization as well as the fact that nature and man-made products consist of discrete organizations, however, we can come up with a very clever resolution to overcome the above seemingly formidable difficulties.

4. Macro-Micro Interlocked Algorithm

As is shown in Fig. 1, a system usually consists of plural, not more than 5, organizations (layers) in spatial and temporal scale domains and the intermediate (gap) region between neighboring organizations is a void region where no active information and energy are in existence. Thus, the void region may well be disregarded in the simulation of the system, which drastically reduces the load of simulation. Hence, the temporal and spatial scale domains could be drastically reduced, if lower (microscopic) processes are dynamically solved at each, say, grid point of the upper (macroscopic) spatial domain and at each macroscopic time step. This reminds us of an idea that the macroscopic simulation and microscopic simulation be done with their own simulators independently and that the information exchanges be done only at each macroscopic grid point with the connected microscopic processor (simulator) (see Fig. 2).

Even if such an algorithm solving simultaneously macro and micro processes be chosen, yet the situation is





Fig. 1 Any system consists of two or a few internal systems(organizations or layers). Each layer is distinct in scale and information (energy) in each layer is mostly confined within 10^4 in scale. When the system consists of two layers, then the total scale is 10^8 or larger since there is a gap scale in between



Concept of Macro-Micro Connection

Fig. 2 A naive conceptual design of two-layer (micro-macro) system

far beyond the horizon of the technical feasibility of High-End-Computing. This can be easily understood by seeing Fig. 2 where required are microscopic processors as many as the number of macroscopic grid points, which is, say, of the order of billions or so. Therefore, we are forced to give up this scheme.

But, we do not have to be so pessimistic. Nature is not so ill-behaved. Imagine, for example, the attack of earthquake. It is really a result of microscopic crust destruction.

However, the crust destruction would not occur spontaneously without any change in its environment. Prior to the fault breakup, energy accumulation proceeds gradually there and the breakup is triggered when it goes beyond the critical point.

Typhoon can be grown up when water vapors evaporated from the equatorial hot sea surface ride updrafts at low pressure region. Thus, in order to predict heavy rainfalls associated with the typhoon development, required is that spontaneous microscopic raindrops formation including rain condensation, fusion of raindrops by collision process and gravitational fall are altogether solved in association with global climate change simulation.

In many energy explosion phenomena that occur in space and universe such as solar flares and galactic jets, environmental evolution of magnetized plasmas forms locally a magnetic field configuration where electron and ion microscopic interaction triggers collision free magnetic reconnection. Once microscopic processes develop sufficiently that such changes can change the ensuing macroscopic evolution, which can again causes drastic changes in microscopic processes, maybe, in different locations. Also, in full automobile design we are required to solve self-consistently and simultaneously the mechanical dynamics including transmission, wheel, handling, etc. and the engine combustion process which are governed by different dynamical equations. In this example, different processes exchange energy continuously through a fixed contact point (boundary).

In most other fields like bio-science, nano-material, nuclear fusion, etc., similar discrete macro-micro feedback processes are taking place. This consideration has led me to come up with a really clever algorithm of drastically reducing the number of macroscopic processors, because at most macroscopic grid points where no drastic change in microscopic state (phase transition) would occur we do not have to make microscopic simulations. Only at specific macroscopic grid points where microscopic instability, phase transition or catalytic action is about to occur, microscopic simulation should be carried out in parallel. Consequently, we can drastically reduce the number of microscopic processors, say, from billions to one or few. This situation is depicted in Fig. 3. Concept of Macro-Micro Interlocked Algorithm



Fig. 3 A conceptual design of the macro-micro interlocked algorithm

5. Concrete Demonstrations of Macro-Micro Interlocked Simulations

Let us show two examples. The first one is aurora formation resulting from double layer acceleration at high altitude field-aligned regions above the aurora region in self-consistent collaboration with the magnetosphere –ionosphere Alfven wave feedback instability [5, 6]. The second example is heavy rainfalls resulting from microscopic dynamical simulation that self-consistently solves the growth and fall of rising water vapors based on condensation and collision processes under the gravity force in self-consistent collaboration with the global climate change simulation resulting in typhoon formation.

5.1 Macro-Micro Interlocked Aurora Formation

It is well known that the original energy source is the solar wind. The solar wind interacts with the geomagnetic field resulting in the formation of the magnetosphere that is roughly balanced between the solar wind pressure and the geomagnetic pressure whereby twin vortices are formed basically in the magnetospheric equatorial plane as is schematically shown in Fig. 4. The clockwise and counter-clockwise magnetospheric convections generate positive charges on the dawn side and negative on the dusk side, which drive field-aligned currents terminated by the ionospheric resistive current. This great current system is unstable for a certain frequency disturbance. Thus, the field-aligned current is locally enhanced. When it grows beyond a certain threshold, the field-aligned current (primarily carried by electrons) interacts with the background ions (protons) and an electron-ion microscopic instability is excited to create double layers, whereby downward electrons are strongly energized to produce excitation of oxygen and nitrogen molecules at the ionosphere. The ionospheric density is also strongly modulated by the local enhancement of ionization, which in turn changes the evolution of the magnetosphere-ionosphere current system (see, Fig. 5).

SUN Solar Wind Micro (particle) simulation F/ectron flow Beattive charges 100,000,000m Macro (MHD) simulation

(Magnetosphere-lonosphere Interaction)

Fig. 4 A conceptual picture of the solar wind-magnetosphereionosphere system in which aurora is excited.

Macro-Micro Interlocked Simulation of Aurora Formation

Solar Wind Global simulation of Magnetosphere-lonosphere feedback instability causing enhan cement of thin field-aligned sheet currents Monitor a location where a field-aligned microscopic instability is likely to occur There, carry out a particle simulation and obtain the energy spectrum of accelerated precipitating electrons Calculate aurora brightening by oxygen and nitrogen excitation by energized precipitating electrons Obtain enhancement of ionization in the ionosphere by energized precipitating electrons

Fig. 5 Flow chart of the macro-micro interlocked simulation of aurora formation



Fig. 6 A shot of aurora brightening seen from the ground (right) and a shot looked down from a satellite (left) obtained by the MMI simulation

Really realistic aurora arcs are generated by this MMI algorithm. Two snapshots (taken from animation) are shown in Fig. 6 [7].

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Formation of aurora arcs obtained by macro-micro interlocked simulation

5.2 Macro-Micro Interlocked Rainfall Formation

In the present simulation of climate change, macroscopic atmospheric and ocean circulations are solved based on Navier-Stokes equations. However, cloud formation is not solved by means of first principles. They adopt so-called parameterization, or at best microscopic physics-oriented parameterization which adds more sophisticated parameters such as several states of water (raindrops, snow flakes, etc.) and spatial distribution



Fig. 7 Flow chart of the MMI simulation of raindrop formation

within each macroscopic grid volume. It is a static model, though, where neither raindrops nor snow flakes formation is dynamically solved. No matter how nicely parameterized, therefore, dynamical causality of raindrops formation is not involved. In order to make a more realistic prediction of rainfalls at a local region, the atmospheric dynamics and raindrops (snow flakes) formation are requested to be solved simultaneously.

In this demonstration a global climate change simulation is done by a newly developed non-hydrodynamic world-fastest global simulation code with 5.5 km resolution [8]. A typhoon is generated and passing over the Japan Island. On the other hand, developed is a new raindrop growth simulation code that solves self-consistently the growth of water vapor due to condensation and collision processes and gravitational fall [9]. By rather arbitrarily choosing a low pressure position in the typhoon rain band predicted by the global code, we give the environmental condition obtained by the global code to the raindrop formation code and obtain how heavy rainfall (see Fig. 7). One preliminary example of rainfall associated with the typhoon at a rain band position is shown in Fig. 8.



Fig. 8 Growing raindrop by condensation and collision processes in an updraft and rainfall when the gravitational force overcomes the updraft force (right) at a certain rain band position of the typhoon arm (left) obtained by global climate simulation with the resolution of 5.5 km

6. Conclusion — Proposal of Macro-Micro Interlocked Simulator

The above two examples are just preliminary ones that are made to test the validation of the proposed Macro-Micro Interlocked Algorithm. Nevertheless, these tests clearly validate that the proposed algorithm is eligible to be the next generation algorithm, With this validation I come up with a good candidate for the next generation simulator. Since the macroscopic simulation and the microscopic simulation are carried out independently except for the occasional necessary information exchanges, we provide two best simulators that are large enough to make the macroscopic and microscopic simulations in self-sufficient manner. Those simulators can not necessarily be the same. One can be the vector-type and the other can be the scalar type. Since both can be of different type, we provide a simple data exchange device that can transfer necessary information on both ways occasionally when the programs running on both simulators give an order to do so. The required demand for this device is about the latency. The latency must satisfy that the intervening time for data exchange is at worst smaller than one macroscopic time step. Another requirement is that the microscopic simulator should have a good performance to ensure the completion of the microscopic simulation within, hopefully, a couple of macroscopic time steps during which no appreciable change occurs in macroscopic state so that we do not have to worry about the loss of physical validation of microscopic simulation.

Fig. 9 is a conceptual design of the Macro-Micro Interlocked Simulator we propose for realizing the Macro-Micro Interlocked Algorithm. Suppose that both macro and micro simulators have main memories that can deal with 10^4 grid points in each direction, hence, the total grid points of 10^{12} . Then, the proposed system can do the job equivalent with the job with $10^4 \times 10^4 = 10^8$ grid points in each direction, thus, 10^{24} grid points in total (three dimensions). In other words, the Macro-Micro Interlocked Simulator can do an equivalent job to the simulator that could have the capability of dealing with 10^{24} grid points. As a matter of course, the practical performance be requested to be increased at least proportionally.

In conclusion, if the simulator system proposed in this paper is developed, I am sure that real paradigm shift occurs in simulation and cutting-edge realm of science is opened up, which can lead to a revolution in academia and industry. Any cutting-edge science and technology can gradually invading into the human society to cause a revolution in life style and eventually end up with a paradigm shift in humans' mind. I would call such a society "Simulation Culture".

Hierarchically Interlocked Architecture



Fig. 9 Conceptual design of the MMI Simulator

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