High Performance Computer Methods Applied to Predictive Space Weather Simulations

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Abstract—**Taking advantage of the advent of massively parallel computers, sophisticated solution-adaptive techniques, and recent fundamental advances in basic numerical methods we have developed a high performance, adaptive-scale MHD code capable of resolving many of the critical processes in the Sun–Earth system which range over more than nine orders of magnitude. The development of such models are of increasing importance as the impact of space weather on vulnerable technklogical systems increases, and too, as the severity of space weather increases with the approach of solar maximum. There is an increasing need to develop physics- based, high performance models of the Sun–Earth system from the solar surface to the Earth's upper atmosphere which can operate faster than real time and which can provide reliable predictions of the near Earth space environment based upon solar observations and upstream solar wind measurements. We report on the status of the Michigan adaptive-scale MHD model, which is one effort whose goal is the development of an operational predictive space weather model.**

Index Terms—**Adaptive mesh refinement, magnetohydrodynamic, numerical simulation, space weather.**

I. INTRODUCTION

THE Sun–Earth system is an extremely complex natural system involving many different interacting elements. Today, the science of space plasma physics has matured to the level of being able to describe many of these complex interactions and to model them. A major goal now is to unify our understanding into a more comprehensive mathematical framework that can simulate and predict the properties of this system (space weather).

This goal is made all the more relevant and timely because of the increased need for a predictive space weather model. "Space Weather" has been used to refer to the conditions on the Sun and in the solar wind, magnetosphere, ionosphere, and thermosphere that can influence the performance and reliability of space-borne and ground–based technological systems or can endanger human life or health. For example, satellites experience the disruptive effects of energetic particles and differential electrical charging during various conditions; astronauts are vulnerable to energetic radiation that may occur at space station altitudes; navigation signals from the GPS satellites are affected by irregularities in the ionosphere that occur under some conditions; massive disruptions in electric power distribution systems can be triggered by geomagnetic storms; and the Skylab space station crashed into the atmosphere because of the increased atmospheric drag due to the atmospheric heating and consequent expansion which resulted from several unanticipated severe geomagnetic storms; to name a few consequences of space weather.

To build a predictive, physics-based, space weather computer model, however, requires that we address and solve several difficult problems. It is necessary to integrate and synthesize the work of many scientists in many disciplines. Further, translating this understanding into models capable of representing the large range of scales for critical phenomena in this system requires very advanced numerical technology. In order to produce models that could eventually be utilized to predict space weather for operational purposes, there is also a need to run the models at speeds faster than real time. This requires high performance computing efficiency.

This paper describes the Michigan adaptive-scale MHD model and its application to the Sun–Earth system and our efforts to produce a predictive space weather code. In particular, the code we describe is built to model the entire region from the solar surface to the Earth's upper atmosphere. This requires that we address physical processes which occur over nine orders of magnitude in scale size. The code itself is described in Section II; the application of the code to simulate a coronal mass ejection is described in Section III. A companion paper in this issue, [11], provides additional details regarding the MHD code and our numerical methods as well as our recent results from simulations of the the solar wind interaction with the Earth's magnetosphere.

A. Description of the Sun–Earth System

The Sun's atmosphere, the solar corona, is so hot ($>10^6$ K) that in regions where the solar magnetic field is insufficiently strong, the corona undergoes a rapid expansion, filling all of interplanetary space with a superfast magnetized plasma flowing radially outward from the Sun. As this flowing plasma, which is called the solar wind, passes the Earth, it interacts strongly with the geomagnetic field, forming a bow shock upstream and

severely compressing the field on the dayside of the Earth, and drawing it out into a long, comet-like tail on the nightside. The confined region of geomagnetic field is called the Earth's magnetosphere.

The solar wind not only confines the terrestrial magnetic field within the magnetospheric cavity, but it also transfers significant mass, momentum, and energy to the magnetosphere, as well as to the ionosphere and upper atmosphere. One dramatic consequence of this interaction between the solar wind and the magnetosphere is the generation of the aurora at high latitudes in both the northern and southern hemispheres. Another consequence is the production of a variety of complex electric current systems, ranging from a sheet of current flowing on the magnetopause boundary between the solar wind and magnetosphere, to an enormous ring of current flowing around the Earth in the inner magnetosphere, to currents flowing throughout the ionosphere and connecting along magnetic field lines to magnetospheric currents systems. Yet another result of the solar-wind/magnetosphere interaction is the production of populations of very energetic particles that are stored in the magnetosphere and precipitated into the upper atmosphere. Both the electric currents and the energetic particles can have severe consequences for a number of human activities being carried out in various locations, all the way from the ground to space. It is the variation over time of these electric current systems and energetic particle populations in the geospace environment that modulates the impact of what we refer to as space weather on various human activities.

The sources of the space weather disturbances observed in the space around the Earth lies ultimately in the sun and its variability. Some geomagnetic storms can be associated with the regular 27 day appearance of long lived coronal holes which are prevalent during the declining phase of the solar cycle and at solar minimum. High speed solar wind from these holes interact with the slower solar wind to produce shock and interaction regions to produce geoeffective configurations of the interplanetary magnetic field. Other storms are the result of large coronal mass ejections in which large regions of dense material are ejected from the sun to form huge magnetic flux ropes which may interact with the Earth's magnetosphere. A major problem is to determine the evolution of solar produced disturbances as they move from the solar surface and to determine if and when they will impact the terrestrial magnetosphere, and to predict the form of the disturbance at the Earth to determine the degree of mass, momentum and energy transfer to the magnetosphere and the associated space weather which would result.

Time scales important to space weather range from minutes to decades. The longest time scales that are usually considered important to space weather are the 11-year solar activity cycle and the 22-year solar magnetic cycle (Fig. 1). Near the minimum of the solar activity cycle, the solar wind is nearly completely dominated by a quasisteady outflow, although there are occasional ejections of plasma and magnetic field from the near-equatorial sun where the plasma is generally confined by the magnetic field. These so-called coronal mass ejections (CMEs) expand into interplanetary space and become integrated into the overall solar wind flow, but they are characterized by closed magnetic field structures oriented nearly perpendicular to the ecliptic plane, in contrast to the background solar wind magnetic field, which on the average lies very nearly in the ecliptic plane. The magnetic field structures associated with these CMEs, called magnetic clouds, as well as their generally enhanced dynamic pressure (ρV^2, where ρ is the mass density and V is the bulk velocity), lead to a significantly stronger interaction with the magnetosphere than that exhibited by quiet solar wind. The major mechanism for energy coupling between the solar wind and the magnetosphere is magnetic merging on the dayside. This is substantially enhanced when the interplanetry magnetic field (IMF) contains a component antiparallel to the Earth's magnetic field, i.e., southward. The CME interaction with the magnetosphere is illustrated in Fig. 2. The magnetic cloud generated by the CME approaches the quiet magnetosphere in the top frame. In the bottom frame the cloud initiates a stronger interaction, which generates stronger magnetospheric current systems and larger, more energetic magnetospheric particle populations a phenomenon which is called a geomagnetic storm. As solar activity increases, the frequency of CMEs is substantially increased, and the "severity of space weather" is concomitantly increased.

II. ADVANCED NUMERICAL MHD MODELING

Developed with support from the NASA High Performance Computing and Communications and from NSF, the University of Michigan adaptive-scale MHD code was designed from the ground up to capitalize on modern numerical methods, solution-adaptive techniques, and massively parallel implementation. The Michigan code, whimsically called BATS-R-US for (Block Adaptive-Tree Solar-wind Roe-type Upwind Scheme), has been used successfully to simulate the environment from the solar surface to the top of the Earth's upper atmosphere.

The BATS-R-US code is based on a high-resolution scheme for the ideal MHD equations [1]. The two pieces of the high-resolution scheme are a MUSCL-type limited linear reconstruction [2]–[6] and a flux function based on an approximate solution to the MHD Riemann problem [7], [8]. This combination yields a scheme that is second-order accurate away from discontinuities, nonoscillatory near discontinuities, and robust across a wide range of plasma parameters. Details of the implementation are provided in a companion paper in this issue [11].

Solution adaptation is a powerful tool for resolving a problem with disparate length scales. By using a solution-adaptive grid, one can avoid under-resolving high-gradient regions, or, conversely, over-resolving low-gradient regions at the expense of more critical regions, and thereby save several orders of magnitude in computing resources for many problems. Length scales in the Sun–Earth system range from tens of kilometers in the ionosphere to the Earth–Sun distance (1.5×10^{11} m); time scales range from a few seconds near the Sun to the expansion time of the solar wind from the Sun to the Earth ($\sim 10^5$ s). These problems need solution-adaptive schemes—a simple Cartesian mesh would grossly under-resolve much of the problem, while over-resolving relatively uninteresting regions.

The approach to adaptation taken in the BATS-R-US code is one of self-similar adaptive blocks [9]. This approach was designed with performance on massively parallel machines in
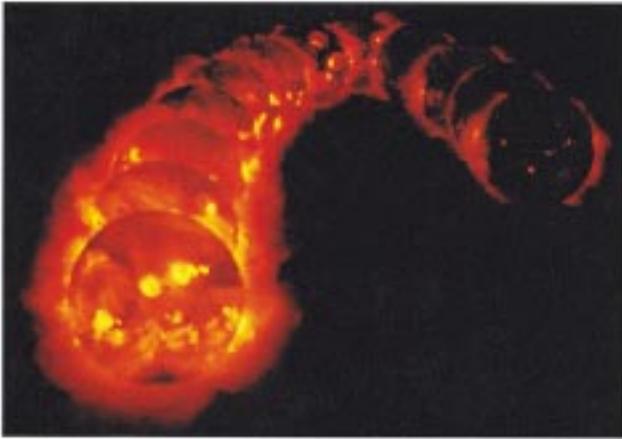
Fig. 1. The 12 X-ray images of the Sun obtained by the Yohkoh satellite between 1991 (left) and 1995 (right) at 90-day increments provide a dramatic view of how the solar corona changes from solar maximum to solar minimum. As we approach solar maximum anticipated in 2001 or 2002, the reverse progression will occur. (Figure courtesy of Lockheed Martin.)

Fig. 2. The interaction of the magnetosphere with an expanding magnetic cloud. (Illustration courtesy of the NASA International Solar Terrestrial Program.)

mind. The basic unit of data is a three-dimensional block of grid cells. A block has a size that is set at run-time; a typical block might have $8 \times 8 \times 8$ cells. The data in the block are stored in i, j, k-indexed arrays, a data structure that is conducive to high cache performance. The code is designed to optimize serial performance on single processors of the target machine while the overall adaptive block scheme also reduces communication to provide high parallel performance. An initial grid is composed of a number of blocks, all at the same level of refinement. Then, in regions that appear under-resolved (as defined by suitable adaptation criteria), a block is refined—each of its eight octants becomes a block with the same number of cells as the original block. In regions that appear over-resolved (again, as defined by suitable adaptation criteria), eight blocks can be coalesced into one. As an example we show in Fig. 3 a two-dimensional (2-D) cut through the three–dimensional (3-D) grid taken from a calculation of a coronal mass ejection [10].

Grids like those shown in Fig. 3 go a long way toward resolving the disparate scales in a problem. Each level of refinement in the grid introduces cells that are smaller by a factor two

Fig. 3. Adapted grid in the simulation of a coronal mass ejection. The figure shows a 2-D cross section of the 3-D grid structure (cutting through the CME).

in each dimension from those one level higher in the grid. Typical calculations have 5–10 levels of refinement; some calculations have more than 20 levels of refinement. In the case of 20 levels of refinement, the finest cells on the mesh are more than one million times smaller in each dimension than the coarsest cells on a mesh.

Massively parallel machines entice users with a factor of 512, or 1024, or even more in CPU and memory resources than single-processor machines. Capitalizing on the promise of these resources is, however, not always straightforward. In general, researchers have had very poor luck with "automatically parallelizing" their codes, or, more generally, with porting legacy codes to this class of machines. The method of *domain decomposition*, i.e., the partitioning of the problem by dividing the computational domain into sections and farming the separate sections off onto separate processors, is the most practical approach for many physical systems requiring the solution to partial differential equations. However, codes that were designed with single-processor computing in mind may have inherent limits on their scalability via this approach. For example, such codes may achieve speed-ups for 16, or 32, or 64 processors, but with additional processors, the codes not only fail to speed up, but actually slow down. These inherent limitations can arise from a variety of sources:

- underlying basic algorithms that are global in nature, resulting in high communication costs;
- underlying data structures that are expensive to partition or to update in a parallel fashion;
- underlying processes that are inherently serial.

In order to avoid any of these limitations, the BATS-R-US code was designed from the ground up with parallelism in mind. The underlying basic algorithm that was chosen is highly local in nature, resulting in low communication overhead. The adaptive-block data structures on which the code was built allow easy, natural partitioning of the data, and greatly facilitate load-balancing, a crucial element of truly scalable computing. Thus, most computation is done within a data block and all data blocks look the same to a processor, whether they are a large block or a small block. Balance and efficiency are achieved by partitioning the blocks among the available processors. The
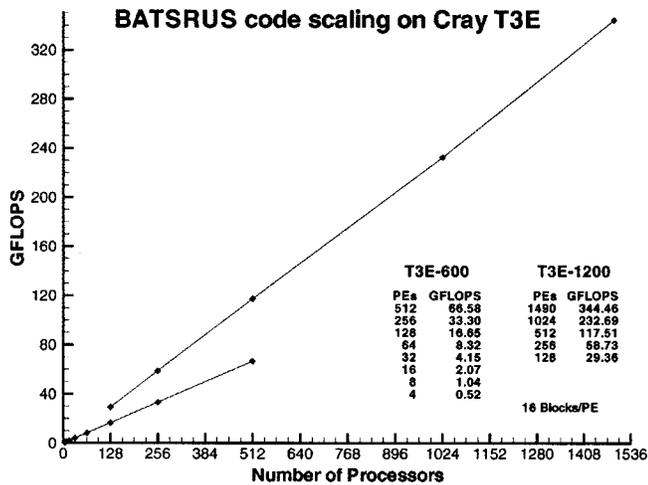
Fig. 4. Parallel scaling of the BATS-R-US code.
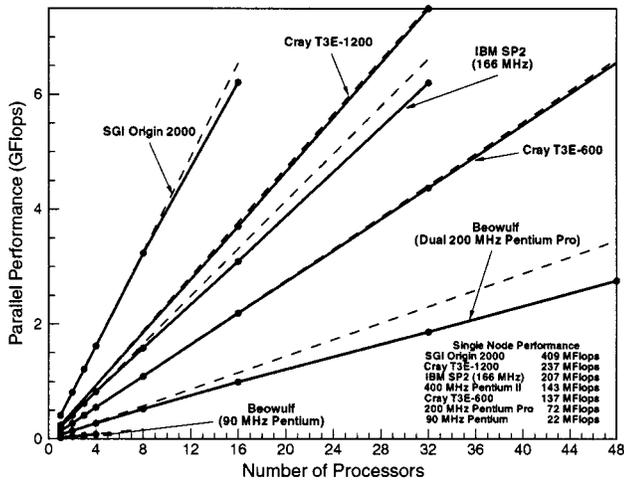
Fig. 5. Parallel performance of BATS-R-US code for a variety of parallel architectures. The dashed line indicates ideal scale-up performance based on single node performance and solid lines indicate actual performance achieved on each of the machines.

design was carried out in such a way that even the adaptation of the grid could be carried out in parallel.

The results of this bottom-up design for scalability are shown in Fig. 4. The figure shows code scaling on two different Cray T3E systems. A fixed problem size per processor of 16 blocks was used. The scale-up for both machines is nearly 100% efficient. Nearly identical results have been obtained on an IBM SP2. The code is written in Fortran 90 with message-passing via MPI, and hence is portable to a wide range of machines, from integrated shared-memory systems to networks of workstations. For each target architecture, simple single-processor measurements are used tune the size of the adaptive blocks. In Fig. 5 we show the performance obtained on a number of parallel architectures without any particular tuning.

III. PROTOTYPE SIMULATION OF A CORONAL MASS INJECTION FROM THE SUN TO THE EARTH

The BATS-R-US high performance adaptive-scale MHD code has been successfully applied to the description of several

solar system plasmas, including the expansion of the solar wind from the base of the solar corona to heliocentric distances well beyond the orbit of Earth and the global terrestrial magnetosphere. A schematic representation of the physical domain described by the Michigan MHD model is shown in Fig. 6.

In the solar wind simulation the source region of the solar wind (the base of the solar corona) is located at 1 R_s (solar radius). The boundary conditions describe a hot, rotating plasma reservoir with an embedded multipole field (up to octapole). The sum of the ion and electron temperatures is 3.1 million K, the magnetic field at the solar pole and equator are 8.4 G and 2 G, respectively, and the plasma density is 10^8 cm^{-3}. Since the physical mechanism of coronal heating is still not understood, the expanding solar corona is heated by an empirical heat source function near the Sun. The specific heat ratio in the simulation is 5/3, thus effects of adiabatic cooling are properly accounted for in the simulation. The resulting solar wind corresponds to solar minimum conditions. The simulation result is quite realistic: it reproduces fast solar wind (~ 800 km/s) above ~ 30 deg heliolatitude, slow (~ 400 km/s) solar wind near the solar equator, and realistic magnetic fields, temperatures and densities near the orbit of the Earth.

The BATS-R-US code was also used to simulate the formation and evolution of coronal mass ejections (CME) in the heliosphere. In this simulation a spatially and temporally localized isothermal density pulse was introduced at the Sun (just above the solar equator). In this enhancement, the density and pressure are locally increased by a factor of 135 in a small region above the solar equator for a duration of 12 hours. The resulting CME rapidly moved through the near solar region and formed a structure which evolved and propagated outward passing the orbit of the Earth. Fig. 7 shows a representation of the magnetic field configuration 9 h after the initiation of the CME. The color code represents $\log(B)$, white lines are open magnetic field lines, magenta lines are closed with both ends connected to the sun. The density enhancement first leads to the "filling" of the closed magnetic field lines with additional plasma and subsequent expansion of the closed field region. One can see that the closed field lines become become stretched by the outward motion of the plasma. This is because the plasma β (the ratio of the kinetic and magnetic pressures) is quite large and the magnetic field is "carried" by the outward moving plasma. Note also the decrease of magnetic field strength behind the leading edge of the outward moving disturbance.

The magnetosphere is an intricate system with the interplanetary magnetic field (IMF) playing the fundamental role in the control of the large scale topology. The magnetospheric topology in turn controls the entry of mass, momentum, energy, and magnetic flux into the magnetosphere from the solar wind. The entry of these physical quantities from the solar wind into the magnetosphere produces various transition layers, the extended geomagnetic tail and plasma sheet, various electrical current systems, charged particle precipitation, and auroral phenomena.

Global three-dimensional MHD simulations have been used to investigate the response of the magnetosphere-ionosphere system to the solar wind and to study a wide variety of processes. A few recent studies include [12]–[19]. Here, however,
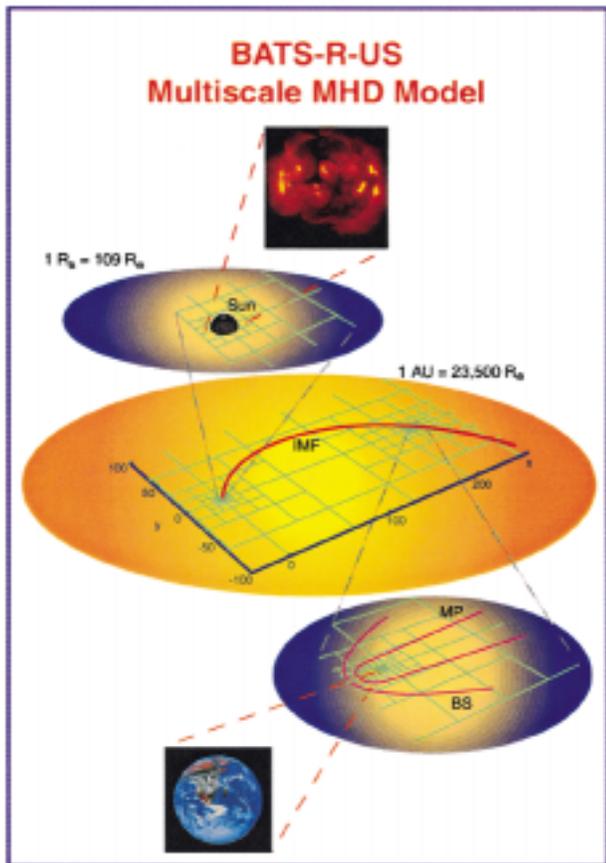
Fig. 6. The Michigan MHD Model. Note that the model spans multiple scales, from a few hundred kilometers in the ionosphere to the radius of the Earth (R_e), to the radius of the Sun (R_s), to the Sun–Earth distance (AU).

Fig. 7. Simulation of a coronal mass ejection (CME) illustrating the 3-D adapted grid structure to resolve multiple-scale phenomena. Magenta lines represent compressed closed field lines ahead of the CME, while white lines show the distorted structure of open magnetic field lines. The color code represents $\log(B)$.

Fig. 8. Simulated solar wind parameters at the Earth—Dashed lines: without CME, solid lines: with CME.

for the first time we have examined the dynamic response of the global magnetospheric configuration to changing solar wind conditions self-consistently simulated all the way from the Sun to 1 AU.

The solar wind changes at the Earth's location result from the rotation of the tilted multipole solar magnetic field and from the passage of the coronal mass ejection. Fig. 8 shows the time evolution of the simulated solar wind parameters as they would be measured by a spacecraft located just upstream of the sub-solar bow shock. The coordinate system used here is Earth centered with the x axis pointing toward the Sun, the z axis pointing North and y completes a right-handed system. For this simulation the Earth is not rotating and the magnetic dipole is Earth-centered and perpendicular to the Earth–Sun direction.

The first signatures of the CME are seen in the magnetic field components at around 55 h after initiation. The driving mass (piston) arrives around 72 h after initiation. The B_x and B_y components exhibit a significant rotation around the y axis—the signature of the passage of a CME-related flux rope or magnetic cloud.

Fig. 9 shows the change of the global magnetospheric configuration during the passage of the CME. Four 3-D snapshots at $t = 70.5$ h, 78.5 h, 86.5 h, and 94.5 h. The color code represents the electric current density in the equatorial plane, solid lines show last closed magnetic field lines. The global magnetospheric configuration is primarily controlled by the IMF

Fig. 9. The response of the magnetosphere to the CME.

B_z component. For $B_z < 0$ the magnetosphere exhibits an open configuration with significant dayside reconnection between IMF and geomagnetic field lines. For strong northward IMF conditions ($B_z > 5$ nT) the magnetosphere becomes practically closed with magnetic reconnection limited to small regions above the cusps. For this CME simulation, the resulting IMF at the Earth is not particularly "geoeffective" since the IMF B_z component is northward with intermediate values between

0 and 3 nT. The global magnetospheric configuration does not become pure "South" or "North". However, the magnetosphere changes significantly during the event. As the solar wind dynamic pressure increases, the dayside magnetopause moves inward and the current density increases. In addition, the magnetosphere becomes narrower and the length of the magnetic wings increases from about 60 R_E to 90 R_E. Overall, the energy and magnetic flux stored in the magnetosphere also increase substantially. Another interesting feature is the clockwise "twist" of the magnetosphere perpendicular to the solar wind direction. The twist, which is particularly visible in the wings, is due to the presence of the nonzero IMF B_y component. A more detailed and complete description of the CME simulation is presented by [20].

IV. CONCLUSIONS

Continued research into the development of high-performance numerical algorithms combined with the continued development in high-performance hardware will make it possible to achieve a predictive space weather model in the near future. The present Michigan code has been run on a Cray T3E with 512 processors and has achieved performance at about 2 times faster than real time using 2 million cells in the CME simulation for the entire Sun–Earth system. However, for operational and realistic space weather purposes, considerable improvement must be achieved. Much greater resolution, requiring approximately 10 million cells, is required, and the code must achieve 2 times faster than real time on a more modest machine, say 16 or 32 processors. Further, the code requires a number of improvements in the physics. These include a more realistic ionosphere and upper-atmospheric model, rotating Earth with a tilted dipole, as well as the inclusion of a model of the inner magnetosphere where the radiation belts and ring current are significant space weather features during magnetic storms. Thus, the challenge over the next few years is to improve the computational performance by about a factor of 100 while also including more complete and increasingly complex physical processes. Some of the anticipated performance improvement will be accomplished by improvements in computational hardware capabilities, and further improvement will be accomplished by improvements in our numerical algorithm technology and software design.

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He is a member of the American Institute of Aeronautics and Astronautics, American Geophysical Union, Society for Industrial and Applied Mathematics, and Canadian Aeronautics and Space Institute. In recognition of his graduate achievements, Prof. Groth was the 1991 recipient of the G. N. Patterson Award and a 1992–93 University of Toronto Governor General's Gold Medal.

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Dr. Holzer received the James B. Macelwane Award of the American Geophysical Union in 1978, is a Fellow of the American Geophysical Union, and was inducted into the Norwegian Academy of Science and Letters in 1995.