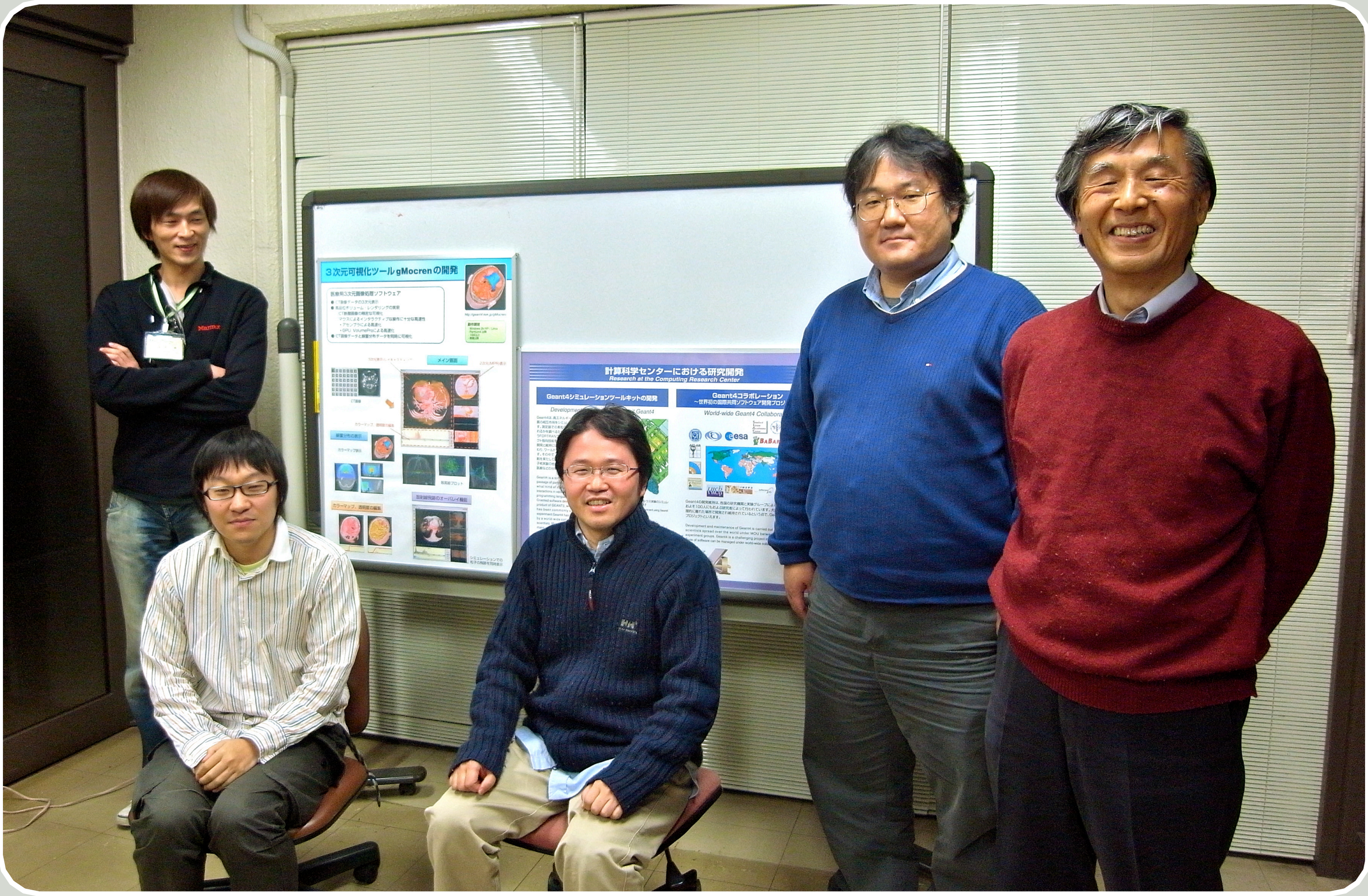
April 28, 2010

FEATURE STORY



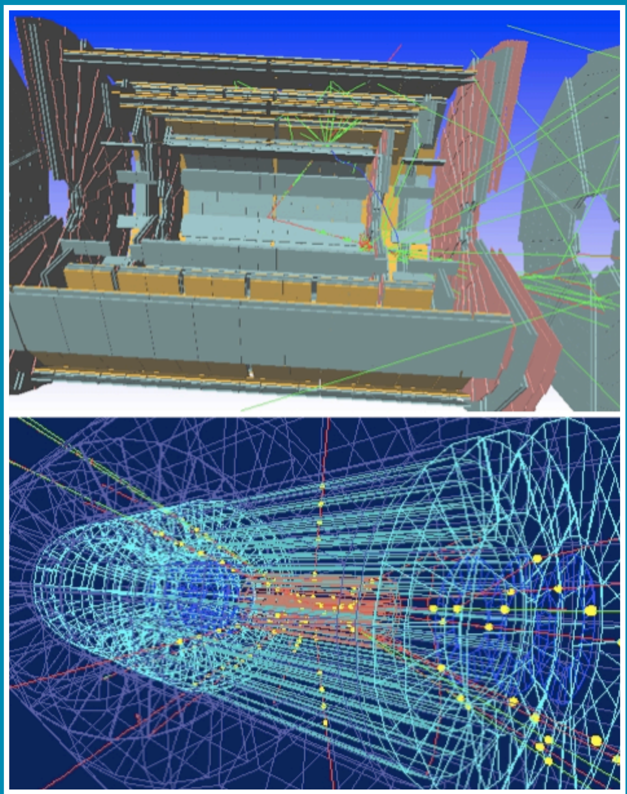
Particle simulator reaching out

One of the world's most powerful particle simulators, Geant4, has helped simulate particles in large-scale particle colliders worldwide for over a decade. Its versatility and scalability have also gathered attention from fields beyond particle physics. Read here about the origins of Geant4 at KEK, its decade-long development by an international collaboration, and its recent application to real-world problems in medicine and space science.

The KEK's Geant4 group is the co-founder of Geant4, and the original developers of Geant4's components. From right: previous leader of KEK Geant4 group, KEK Diamond Fellow Prof. Katsuya Amako; the current KEK Geant4 group leader, Prof. Takashi Sasaki; Dr. Koichi Murakami; Dr. Chihiro Ohmachi; and Dr. Go Iwai.

The object-oriented style of programming was just starting out in the early 1990s. Around the same time, scientists were developing proposals for several different mammoth particle colliders. The existing particle simulator, GEANT3, needed an upgrade to handle the immensely complicated many-particle interactions that would be taking place in the extreme high energy environments created by the proposed colliders. Prof. Takashi Sasaki, then a graduate student and now the head of the Geant4 group at KEK, was learning about object-oriented programming from his supervisor. Right away, he and the team lead by Prof. Katsuya Amako from KEK, and including several universities in Japan, started exploring the potential of a new particle simulator written in an object-oriented programming language.

"Although Geant4 is the spiritual successor of the Geant series of simulators developed at CERN, it is an entirely different simulation platform from any of its precursors," explains Sasaki. "The main problem with Geant3 was that no documentation on its program design was available. Only, say, ten people in the



Geant4 is a simulation toolkit primarily used in the field of high energy particle physics experiments, and has been utilized by many experiments around the world. The images above show simulation results for the Large Hadron Collider’s ATLAS experiment at CERN. (Photo credit: http://atlas-computing.web.cern.ch/atlas-computing/packages/simulation/geant4/photoGallery.htmls)

world knew how it worked.” Additionally, GEANT3 was written in FOTRAN, which is a procedural programming language. The extremely complicated nature of the simulation code, and the relative lack of structure inherent in most procedural languages, made it impossible for general users to add new components to the program.

Geant4 is written in C++, an object-oriented programming language. “The object-oriented style allows us to separate each function and component so that users can add their own functions without having knowledge of the rest of the toolkit,” says Amako. The design is simpler, has better organization, and better documentation.

The scalability of Geant4 brings significant advantages. From the very beginning, the team was well aware of this. Among these advantages, Geant4 is currently the only particle simulator that can simulate every kind of interaction on every type of radiation across a broad range of energy levels. This means that Geant4 can be used for simulating the effects of proton beam and carbon beam on organic molecules, something which is important in particle cancer therapy. On the other hand, it can just as easily be used to understand the effects of harsh radiation on the human body in space. “While developing the core components, we made sure that Geant4 could be extended to include any potential fields that deal with radiation,” says Sasaki.

According to the project webpage, Geant4 is open-source Monte Carlo software “for the simulation of the passage of particles through matter.” As with its precursors, Geant4 is freely downloadable from the project site.

To simulate the passage of particles, Geant4 contains a wide variety of information and algorithms. For example, it includes geometrical and functional information about detectors, procedures to simulate possible interactions and decay processes of particles, and a Monte Carlo generator to deal with the probabilistic nature of quantum mechanics. Geant4 also provides tools for run management, visualization, and user interface.

The international Geant4 collaboration

The object-oriented simulation project at KEK was originally called Prodig. Dr. Yoshinobu Takaiwa of KEK, Dr. Junichi Kanzaki of KEK, Amako, and Sasaki were the Japanese gang of four. They were responsible for the design and development of a prototype particle simulation tool for the Superconducting Super Collider (SSC), a proposed 40 TeV hadron collider in the US. When the SSC plan was cancelled the following year, the team needed another project to work on.

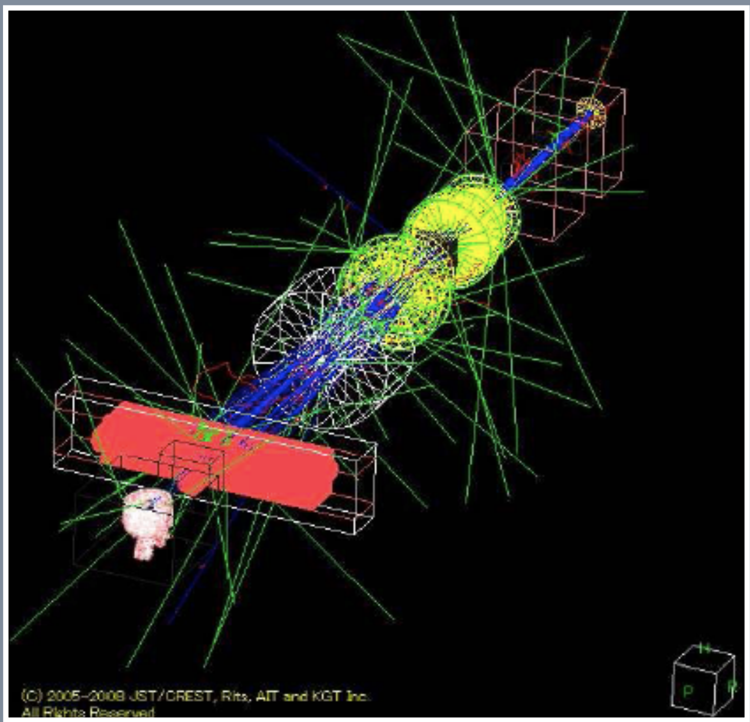
In 1994, scientists working on another proposed hadron collider, the LHC at CERN, became interested in Prodig. The result was that the Geant4 collaboration was officially started at CERN. The collaboration quickly grew to include many nations. Amako, Sasaki, Prof. Hisaya Kurashige at Kobe University, Dr. Makoto Asai at SLAC, Prof. Hajime Yoshida at Shiokoku University, and Prof. Satoshi Tanaka at Ritsumeikan University were joined by others from TRIUMF in Canada, INFN in Italy, IN2P3 in France, SLAC in the US, and many others.

The European Space Agency also recognized the potential of Geant4, and joined the collaboration in 1996. With the ability to simulate all types of radiation with a wide range of energy, Geant4 was ideally suited for use in space science, for the simple reason that space is filled with all sorts of radiation. The relatively easy way in which new parts could be added to the software allowed for complete simulation of the way in which radiation would affect both spacecraft and the human body.

By 1996, the Japanese group had finished the complete core components of Geant4. This included everything where the physics of radiation was concerned. However, this was just the start. Eventually, Geant4 was expected to include all possible physics, covering electrodynamics and nuclear and hadron physics for all types of radiation. To do this, the Geant4 team needed to collaborate closely with experts from every possible field in physics.

With help from overseas collaborators, the first release hit the world in 1998. Since then, the collaborators have been actively improving the

Geant4’s applications are many. The international collaboration of Geant4 was joined by the European Space Agency (ESA) in 1996 to simulate the effects of radiation on spacecraft and the human body in space.



Another Geant4 application includes radiotherapy simulations. The detailed simulation of the complex processes of fundamental physics helps doctors predict the precise consequences of cancer treatment by radiation.

base code, improving both function and speed.

How Geant4 can save people

This past decade, the team has been working to make Geant4 available for medical use. Funded by the Core Research for Evolutional Science and Technology (CREST) program at the Japan Science and Technology Agency (JST) from 2003 to 2009, the team worked closely with medical research centers in Japan to develop a Geant4-based simulator for radiotherapy.

Radiotherapy uses many types of radiation in order to cure cancers. Types of radiation include electromagnetic radiation (such as gamma-rays and X-rays), beta particles, neutrons, and ions (such as carbon and protons). It is relatively easy to simulate electromagnetic radiation, as it involves only one of the four basic forces: the electromagnetic force. Simulating ions requires the inclusion of additional forces, and is harder. Before Geant4, there was no simulation tool that could handle all of these interactions.

The team faced a number of challenges in adapting Geant4 to medical use. The first challenge involved geometry. The digital imaging and communications in medicine (DICOM) interface would read in the patient geometry data from CT scan. The data structure of CT required the design of a new data handling scheme. In particular, the data was organized as a set of boxes. The boxes from the CT were 5x5x5 cubic millimeters. While interactions in water can be calculated using a much longer distance scale, the CT data structure required Geant4 to deal with physics every 5 millimeters. This slowed the speed of the calculation. To optimize the performance of the software, the team tried many different geometry implementations.

The second challenge was particle energy. Because Geant4 was primarily built for high energy physics experiments, the behavior of ions at the lower energies used in radiation therapy had not been properly implemented. High energy physics experiments passed the 500 MeV level long ago, and crucial data about low energy behavior were long lost or not digitalized. Therefore, expanding the energy to the fullest scale was also an important mission of the team.

The successful Geant4 software allowed radiotherapists to simulate their medical treatment without requiring real samples. Before Geant4, no simulation came even remotely close to the experimental results. “The Geant4-based radiotherapy simulator gave a match with the experimental results with just few percentage error. Previously, no theoretical prediction was possible. The difference is that Geant4 simulates every fundamental physical process, while previous simulators which doctors had used were based on very simple models and approximations,” says Sasaki.

The new Geant4 medical toolkit is equipped with a fabulous user interface in which radiotherapists can maneuver their operations and examine the results in informative full 3D.

The program was completed last year, and the team is now tackling the next issue: speed. “With 20 CPUs, the software takes one night per run. Doctors need it in less than a minute. We are now working on several new technologies that enable faster computing,” says Sasaki.

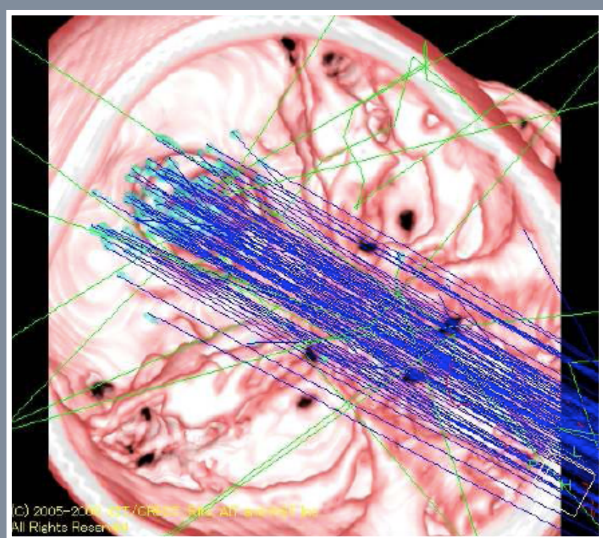
Speeding up Geant4 with the help of the world

The current Japanese Geant4 team includes five researchers at KEK, six from universities and one from two radiotherapy research centers in Hyogo and Chiba. The team is currently working on several tasks. These include software management and user support, development of new functions, and improvement of the base code.

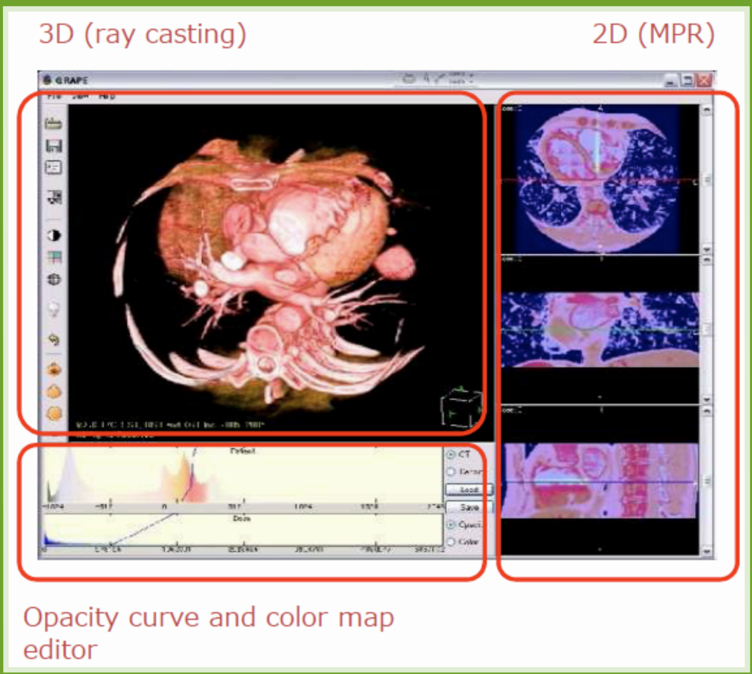
“One job of critical importance is to speed up the run time. Faster is always better, but for medical users who need diagnoses as precisely as possible and as quickly as possible, run time become a crucial issue,” says Amako.

“Hospitals are generally closed, small places, while the Geant4 simulation requires very large scale computing capabilities and CPU time,” says Dr. Go Iwai who leads the GRID effort at KEK. GRID is a new technology that allows sharing of data and massive CPU power distributed around the world. By taking advantage of the unused resources of distant computers, Geant4 users can run a simulation in a drastically shorter period of time. Using GRID, “a radiotherapy simulation run will take no more than a few tens of minutes, instead of a whole night,” says Sasaki.

The team thinks beyond GRID. By combining the GRID technology with a web portal, the



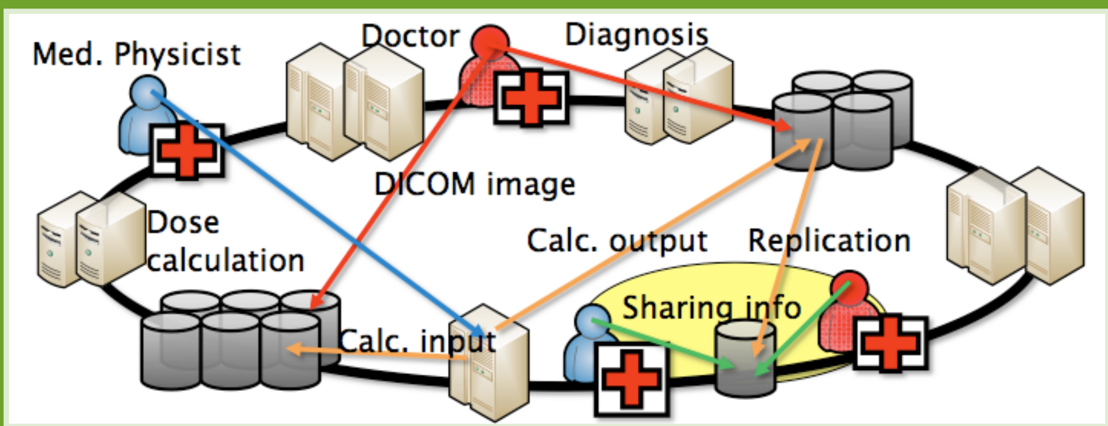
A brain tumor treatment is being simulated.



Using the gMocren interface to Geant4, doctors can treat cancers and get results in 3D.

technology offers an entirely new possibility to connect the world of high energy physics and our lives via web. Iwai had developed a test GRID web portal for radiotherapy simulation. Medical physicists can go to the web portal site, input information in fields, and click run. The simulation will run in the background using CPU resources from around the world, and give back the results on the website. Iwai plans to develop web portals for fields where demand is high to bring the 3D simulation of complete radiation physics just a click away.

A second new technology, one which was introduced just a couple of years back, is the ability to use the graphics processing units (GPU) on desktop graphics cards for general purpose computing. According to Dr. Koichi Murakami of KEK, who conducts R&D into parallel computing for Geant4, “Using GPU technology, we are exploring the possibility to implement parallel computing ability in our Geant4 codes.” Murakami will have to figure out how to introduce parallelism and GPU technology to software which is 15 years old, and that is not easy. When he succeeds, Geant4 will make another big leap forward, becoming a much faster tool.



To share the resources of computers around the world, scientists use a new technology called GRID. This efficiently uses unneeded resources located elsewhere, and therefore speeds up computation dramatically.

Connecting to society

Although Geant4 is a completed toolkit that has been vastly successful, the team continues to improve the base code and to adapt the software for fields beyond Geant4’s original scope. With the introduction of a new young member, Dr. Chihiro Ohmachi, who just joined this April, the team has many irons in the fire.

Now that they have successfully adapted the software for medical and space science, the team says they would like to do the same for other fields.

The team is now considering the possibility of including human cell structure in Geant4. “Implementing cell structure requires close collaborative efforts with medical researchers and patients,” says Sasaki. “With a computational model of cell structure, we will be able to simulate how the double strands of cancer DNA are affected by radiation. This would provide us with improved biological understanding of how cancers can be healed.”

Another of the team’s current efforts is to expand the Geant4 user community in the world. They have hosted series of workshops for eager researchers from Asian countries such as Korea and Taiwan, to explain what Geant4 can offer. “We are very enthusiastic about welcoming and supporting new users from as many countries and fields as possible,” says Sasaki.

“In general, simulations are perceived as having secondary importance, because they're just a grand sum of what’s already known,” says Amako. “However, to offer what’s truly useful to the society requires complete integration of every aspect of physics and geometry. In that sense, simulation is a comprehensive system of human knowledge. I believe what is really important in the basic science is the ability to contribute to the society.” Geant4 does just that.

Related Link:
Geant4

Paper:
S. Agostinelli et al., Nuclear Instruments and Methods A 506 (2003) 250-303 -- 1,974 times cited!

J. Allison et al., IEEE Transactions on Nuclear Science 53 No. 1 (2006) 270-278 -- 323 times cited!

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