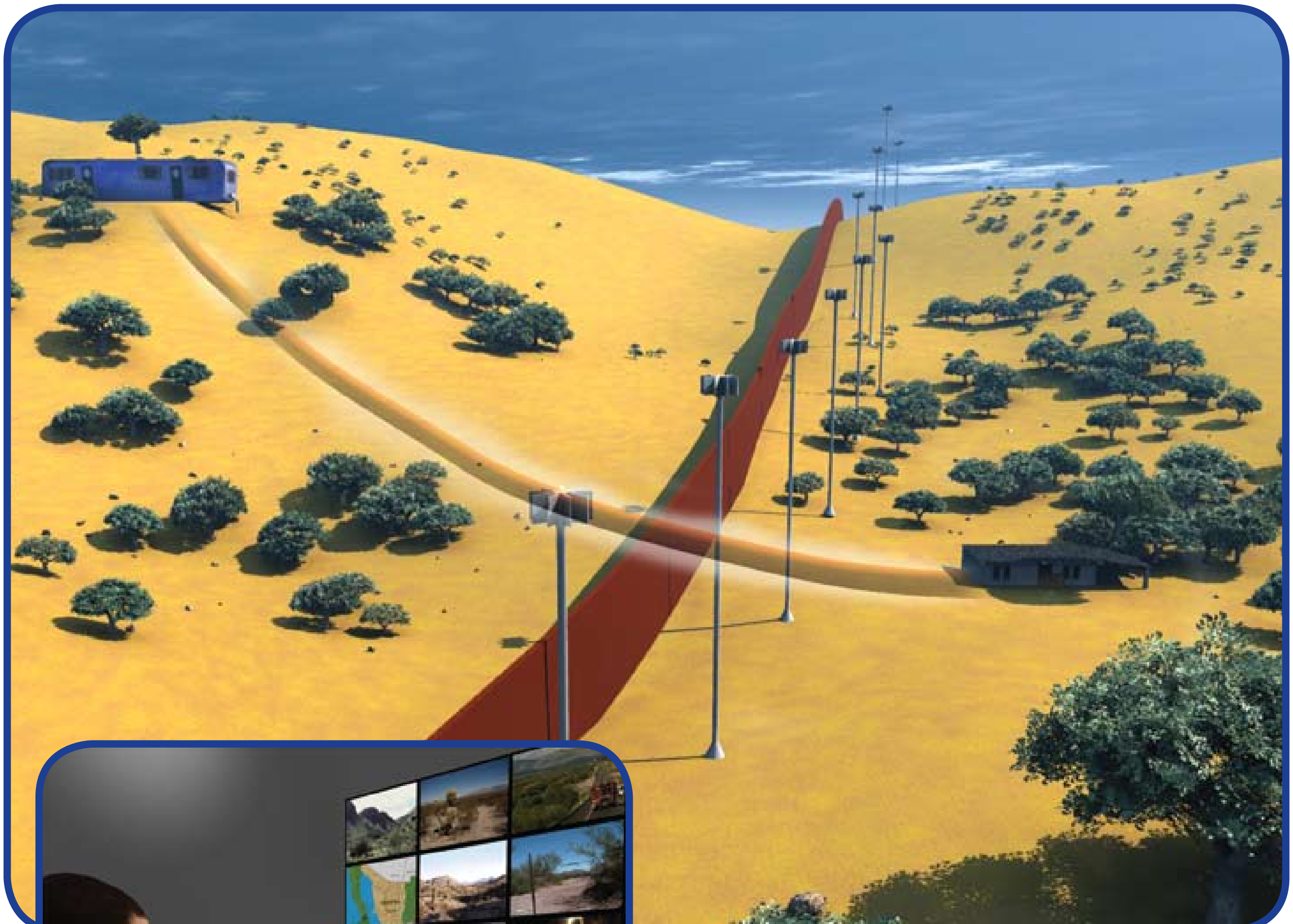
Massive Quantum Research Project Pushes Boundaries

This High Performance Computing Modernization Program (HPCMP) Capability Applications Project (CAP), "Quantum Algorithms for MHD and Turbulent Flows," was run at the AFRL MSRC by Dr. George Vahala, Professor of Physics, College of William & Mary, Williamsburg, Virginia in support of the Hanscom AFB. AFRL MSRC System Utilization: SGI Altix 4700 (HAWK) with 2,251,713 total hours



By Gary Sivak and Dinah Luneke

Border Patrol Scenario

Guards leisurely glance at computer screens to check on results from the continuous scanning for underground disturbances along the U.S.–Mexico border. In this future scenario, thanks to the field applications of Jeffrey Yepez (AFRL) and Dr. George Vahala's work, guards may more easily be able to detect underground movements in order to prevent illegal aliens from slipping into the country. These and other future applications are pushing the boundaries of quantum research as Dr. Vahala and his colleagues work to enhance and expand the capabilities of the DoD in order to serve the warfighter.

HPCMP "Tips Its CAP" for Massive DoD Projects

Memory can mean several things to people for a variety of reasons. Attaining adequate computer memory for DoD research projects elevates this concept to a whole new level for the research user community. In its quest to help DoD researchers fulfill their mission, the HPCMP provides resources for large scale computer runs for its CAP program, which includes goals to:

1. Quantify the degree to which important application codes scale to thousands of processors, including the identification of potential bottlenecks for scaling these codes
2. Enable new science and technology for the DoD by applying these codes in dedicated, high-end, capability environments.

During the time period between acceptance testing and production release, the HPCMP makes select HPC systems available for CAPs. Designated users may test their application codes on a substantial portion of the entire system and solve large, meaningful problems in a relatively short time.

Dr. Vahala was granted a CAP for the TI-07 HAWK system at the AFRL MSRC to run his memory-intensive research project. A massive amount of research was accomplished through this 9,000 processor study. Dr. Vahala's job represents the largest single job to run on the HAWK, lasting almost 25 hours and using 224,663 processor hours.

From CFD to Kinetic Velocity Space

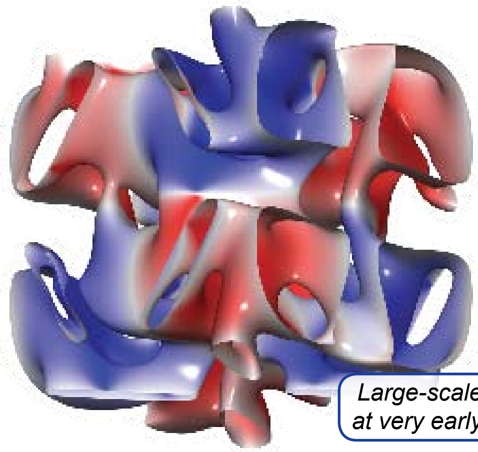
Two distinct projects were part of this theoretical research CAP. The first was a classical project – Magnetohydrodynamics (MHD), similar to the turbulence found on Jupiter and in plasmas, and the second used the quantum lattice approach to quantum turbulence. This massive computer run consisted of homegrown codes that were mesoscopic detail balanced representations. For instance, if fluid or MHD turbulence is observed, the flow is collision-dominated and makes valid the direct Computational Fluid Dynamics (CFD) solution of the continuum equations (like the CFD solution of the Navier Stokes Equation for fluid turbulence).

According to Dr. Vahala, the inherent problem with using CFD codes for such large-scale computer analyses is their scalability with the number of processors. Typically, as more and more processors are added to solve the flow, while working in a CFD code, the simulation run time will merge together. In essence, when doubling the number of processors, one would anticipate that as the numbers go up, the wall clock time – the time one has to wait for the simulation results – should decrease. Instead, with standard CFD codes, after one or two thousand processors, that will cease. The more processors added can actually take longer because the communication between them could result in a road jam.

"The codes that we are running, instead of working in standard X-T space – space/time, go into kinetic space," Dr. Vahala said. "That means more memory, unfortunately. On the other hand, the problem is now in a higher dimensional space and one can get a simpler solution trajectory, which can be solved more simply. Not only that, but you can then parallelize so, in fact, you do not see any saturation with cores. That's why we ran with all the 9,000 cores that were available."

The dimensions used involve space/kinetic/velocity/time, which translates to a factor of "6+1." This simply means, "Six in velocity-space, and one in time." The advantage of the lattice discretization method is that dimensionality in this kinetic velocity space can be reduced. It is difficult to store a six-dimensional array on a computer as the methods are extremely memory bound.

At the time of this writing, Dr. Vahala and his team are "banging at the data analysis" with more than 10 terabytes (TB) of data from a single run.



Large-scale structures at very early times

Pushing the Law of Physics' Boundaries

As this work progresses, Dr. Vahala will continue to seek CAP status at centers throughout the DoD. Besides running at the AFRL MSRC, Dr. Vahala has also run HPC projects at NAVO and ERDC.

"The Air Force chap we're working with is viewing his technique, of these quantum lattice gas methods, as being able to understand the law of basic physics: quantum chromodynamics, quantum electrodynamics, even to unification with quantum gravity," Dr. Vahala remarked. "He has extremely high goals for this method using basic quantum bit (qubit) information where you can obtain the Dirac Equation and others that could result in a unified theory spanning all the fields of study in physics."

MHD equations were modeled during the intensive CAP. These are the basic starting equations for the study of turbulence where conducting fluid or plasma interacts with a magnetic field. Plasma fusion, solar, magnetosphere, astrophysics – all begin with MHD serving as a fundamental equation. While periodic boundary conditions were utilized in these CAP runs, the lattice method readily adapts itself to handling arbitrary boundary geometries (e.g., those generated by Mathcad®) without losing any of its excellent parallelization. One can readily include more detailed structures like yaw grids and other elements.

Benefiting the Warfighter and the World

Although it is still a little early to predict all the outcomes of this MHD work, there are definitely planning and logistics benefits expected from the quantum research. An area, such as the field of cryptography, works by understanding how information can be passed along that cannot be deciphered without possessing the encryption key. Cryptography studies work like Morse Code. The only way to interpret the message is to understand the code. In similar fashion, messages sent using quantum encryptions can only be correctly interpreted if one possesses the special key to decipher the message. This study of quantum cryptography can help make informed decisions for potentially intercepted data. The information would be coded in such a way as to be considered unbreakable, and interception or eavesdropping would be detectable as the interference can be tested.

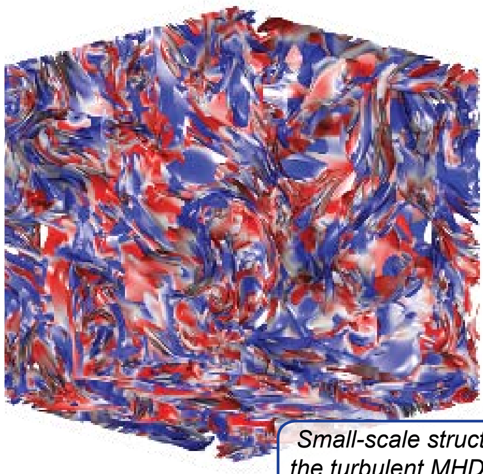
The Beat Goes On

The results of this study have generated a tremendous amount of interest in the scientific community. In analysis, the extremely small fluctuations (10^{-14}) involve a study of interference patterns. This is similar to comparing the difference between two musical tones. Normally, one cannot tell the difference in the beats by simply listening, but if one were to compare them side by side, the differences between the two tones would be much more noticeable.

"There is simply no end in sight for this research as the work is quite continuous," Dr. Vahala said. "If you did not have HPC access, you could not get anywhere, and it's even stronger than that. Without HPC, this work just could not be accomplished. Typically, each processor has only two gigabytes (GB) of memory. So to perform large-scale simulations, one really needs to be able to use the 9000 cores optimally. Our codes do that. This type of research project cannot be performed even with dozens of researchers working side-by-side in a laboratory on PCs. Our research requires the enormous computer capability of such a massive system as the HAWK."

Potential future applications of this work include such areas as: improved weather predictions using advanced ocean modeling; smaller, lighter, and more efficient engines; unbreakable encryption of sensitive information; and the development of next-generation materials for submarines and other military vehicles. ■

For more information, please contact CCAC at www.ccac.hpc.mil or 1-877-222-2039.



Small-scale structures in the turbulent MHD regime