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Computer Simulation and the Comprehensive Test Ban Treaty

by Peter D. Zimmerman and David W. Dorn

Overview

All nuclear weapons now in the American stockpile were developed with the aid of computer models validated by comparison with nuclear tests. However, those models required the use of parameters that were not well understood and often needed adjustment to make computation and test agree. Facing the possibility of a test ban, the Department of Energy initiated a Stockpile Stewardship Project to develop a predictive capability with validated, physics-based simulation tools at its core. This program is charged with maintaining the performance, reliability, and safety of U.S. nuclear weapons without nuclear testing. To meet the requirement for maintaining the enduring stockpile, the Department of Energy engaged the three national weapons laboratories in creating the Accelerated Strategic Computing Initiative (ASCI). ASCI advanced computational capabilities and three-dimensional models, combined with major experimental and testing facilities, should make it possible for the United States to maintain its present nuclear stockpile indefinitely. The authors believe that the ASCI computational capabilities also will enable nuclear weapon designers to draw on archived data from more than 1,000 nuclear tests to adapt proven designs to future mission requirements. Through extensive computer modeling and nonnuclear testing, new nuclear weapons could be designed and introduced into the stockpile, so long as the new weapons used design concepts similar to those proven in nuclear tests.

All U.S. nuclear weapons have been designed on computers. This was true even in 1944–1945, when "computer" was a job title for a small army of young women. Many were the wives of the scientists and technicians designing and building the nuclear weapons. Each of the "computer elements" operated a Marchant or Frieden mechanical calculating machine, entering results of one or two operations on an index card and passing it on. Sometimes the choice of which person to pass the data on to depended on the result of the computer's calculations. The computations required to ensure that a modern nuclear weapon functions as desired are, in general, far too complicated to be performed by a few people armed with nothing but old-fashioned mechanical calculators. As the American experience with nuclear weaponry evolved from the crude devices of 1945 to more sophisticated designs that were lighter and more powerful and used less uranium or plutonium, the need for fast electronic computers grew. Indeed, the nuclear weapons establishment was one of the driving forces behind the early development of computers.

A thermonuclear weapon includes layers of materials, such as uranium and/or plutonium, some kind of tamper or reflector material, a high explosive, boosting gas made up of tritium and deuterium, fusion fuel using lithium deuteride, and an outer casing (radiation case) that encloses the explosive components. One major problem in designing a device is ensuring that the shock waves from the high explosive properly cross the boundaries between layers and that the energy from the primary is properly absorbed by the secondary. Matching such boundary conditions is a

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difficult computational task that is essential to success. Other tasks for the design program include understanding how solid metal is made to flow like a liquid or compress like a gas (that is, solving the equation of state of the material).

Nuclear design codes may be one-, two-, or three-dimensional. That is, they can reduce computations to the minimum by treating each component separately and only examining what goes on along a single line through the primary or secondary (one-dimensional); they can examine a section through the objects (two-dimensional); or they can model the actual three-dimensional shapes of the primary, secondary, and radiation case. One-dimensional calculations are clearly too simplified for modern nuclear weapons; three-dimensional codes stressed the capabilities of the largest computers in the world only a little more than 10 years ago.

the $700 computer under the average desk is at least as powerful as the supercomputers of the late 1980s

In general, nuclear weapons design codes have been used to answer such technical questions as:

- How does the high explosive compress the fissile material?
- How does the nuclear chain reaction in the fission primary begin, propagate, and die out?
- When does "boosting" begin, and when do favorable conditions for boosting occur?
- After boosting occurs, how is energy produced by the primary, and how effectively is it transported to the secondary (the "hydrogen bomb" part of the weapon)?
- Once the energy reaches the secondary, will the second stage function, and with what yield?

The so-called legacy design codes, written before the Department of Energy created its Accelerated Strategic Computing Initiative (ASCI) program and generally before the end of testing, explore the explosion of a nuclear weapon in a simplified manner. They often require the incorporation of adjustable parameters learned from explosive nuclear testing. While the authors of the legacy codes incorporated a great deal of detailed physics in their work, they could not handle many of the phenomena from first principles. The adjustable parameters were in some sense a measure of scientific ignorance about the intimate details of the physics and a demonstration of the inability of the codes of the era to calculate the effects of small changes (for example, in metals, structure, explosive chemistry, and design) that might arise during the fabrication or aging processes.

Due to rapid advances in processor speed, memory speed, and capacity, as well as the development of graphics cards and large hard disks, the $700 computer under the average desk (2001 pricing and specifications) is at least as powerful as the supercomputers of the late 1980s. Two-dimensional design codes similar to the legacy codes can be run on such machines.

Such design codes predict in simplified form what will happen in a nuclear weapon when it functions basically as intended. They cannot include details of nonnuclear components or even such real and necessary features as welds, bolts, and the ancillary plumbing required to make a real weapon. Even the most powerful computers used to design the most modern U.S. nuclear weapons were too slow and had too little memory to handle such complications. Legacy codes ran on supercomputers with speeds in the range of hundreds of mega-computer operations per second (megaOPS) to a few gigaOPS; the new generations of computers used for ASCI have speeds between one and one hundred teraOPS.[1] While the large Cray and other supercomputers of the 1980s and 1990s had random access memories storing a few to a few hundred million bytes of information, the large ASCI machines have already reached 6.2 terabytes[2] of fast memory plus 160 terabytes of disk storage space.

By 2005, the fastest ASCI machine, which will be installed at the Los Alamos National Laboratory, will operate at 100 teraOPS. The purpose of computers with such blazing speeds and gigantic memories is not the raw production of numbers, but, as mathematician R.W. Hamming pointed out, to gain insight into the problem at hand. To this end, a major part of the ASCI effort is devoted to the search for ways to visualize the enormous flow of computed data.

Simulation of the results of time-induced changes in the weapons of the stockpile, combined with an aggressive stockpile surveillance program to detect those changes, is intended to provide the stewards of the nuclear stockpile with the information needed to certify the safety and reliability of the enduring stockpile in the absence of nuclear testing. Before President George Bush's 1992 decision to end U.S. nuclear testing and with it the program to develop new nuclear weapons, a suspected problem in a given weapon could be put to the ultimate test—an underground nuclear explosion. Testing was an option used rarely and generally only with weapons that were already showing unmistakable signs of problems during inspection or as a result of new computations of the behavior of the device. It was, however, available in the case of extreme need and was instrumental in *confirming* suspicions that the WB80 air-launched cruise missile weapon would not perform properly after becoming chilled during a long flight under the wing of a B–52 bomber. The necessary changes were made subsequently.

American designers also did not worry about the performance of very old nuclear weapons. It had been standard practice to retire older weapons from the stockpile as new delivery vehicles carrying new weapons were developed. After the Bush test moratorium was put into place in 1992, development of a new weapon was considered risky because it could not be subjected to a nuclear proof test.

The Role of Verification and Validation

A major goal of the ASCI program is to enhance computational capability so that it can substitute for nuclear proof and safety testing. To give U.S. policymakers the same level of confidence in the

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reliability and safety of the stockpile that they would ordinarily get from nuclear testing, the Department of Energy requires that simulation codes be both verified and validated. Neither verification nor validation is an easy task, but both must be accomplished for ASCI to be effective.

Verification of the code means scientists have determined that the software implements an algorithm that correctly represents a "model of a physical process." It may be loosely thought of as finding and correcting errors in the coding of the program (debugging of code) and running check cases to ensure that the program correctly computes the equations used in specific cases. Possible ways to verify the code include constructing appropriate software engineering audit trails to account for changes in the code and establishing that the computation incorporates correctly the fundamental physics problems. Such problems will include propagation of chain reactions, thermodynamics of the primary and secondary materials, compression of boost gas and the effects on boosting of instabilities in the pit, and the ignition of thermonuclear secondaries. Some of these phenomena are understood well enough to permit physicists to compute limiting cases analytically (that is, with pencil-and-paper mathematics that can be evaluated without using the computer to solve equations), and sometimes exactly. Verification requires that the simulation codes reproduce these known analytical results.

Validation is another problem entirely. It is a process of checking to see that the model represented by the computer code accurately represents the real world, at least in the limited domain of the specific applications. Validation requires the input of measured physical data, the comparison of computational results from the new codes with those of older legacy codes, and comparison with data from actual nuclear test explosions conducted before the end of U.S. testing. Verified code must be validated to show that in the macroscopic world of an actual nuclear detonation it produces results that match data from three sources:

- Legacy codes
- The archived data from more than 1,000 successful and failed U.S. nuclear explosions. Reproducing anomalies, such as primaries that failed to reach predicted yield or secondaries that failed to burn despite proper functioning of the primary, is likely to be a more stringent test for code validation than computing the results of tests that succeeded.
- New data from the Dual Axis Hydrodynamic Radiographic Test Facility (DAHRT), National Ignition Facility, and other facilities giving very detailed information on the performance of specific assemblies that can be built in moderate numbers and tested repeatedly. Such experimental devices can all be built alike, or anomalies such as cracks, deformations, and asymmetries, can be inserted to show the behavior of the device and the simulation systems in detail.

The verification and validation program has passed its first major milestone, demonstrating "initial validation methodology" of the current state of ASCI code modeling for early-time primary behavior.

simulation can also be used to study the behavior of nuclear weapons in abnormal environments, such as fire or plane crashes

Not all validation of the ASCI systems needs to come from nuclear weaponry. The problem-solving environment is applicable to complex problems in many fields. Developers can ensure that the underlying computational structures that translate a problem from language appropriate to a small machine to the massively parallel supercomputer platforms of ASCI are working properly.

Getting the Physics into the System

Until the advent of the early teraOPS machines, the details of the performance of a nuclear weapon could only be checked in what the weapons community called *integral tests* (nuclear test explosions). Over the last 5 years, the speeds of the computers built for nuclear design (including the ASCI machines) have increased by a factor of about 15; the increase over the last decade may be closer to a factor of 50. Random access data storage capacity has increased at least as much in the same period, as has the ability to build large arrays of mass storage devices (hard disks) at affordable cost. These computer advances allow nuclear weapons physicists for the first time to contemplate including accurate models of such processes as corrosion; deterioration of materials; the effects of turbulence and "mix";[3] the effects of small changes in the dynamic properties of materials; and fractures. Measuring the materials properties involved is difficult, particularly at the small distances where previously unstudied problems in nuclear weapons physics may lie. A vigorous experimental program in the properties of highly stressed materials is essential and has already begun. This program will provide the data and validated physical models needed for simulation to be useful in examining the functioning of weapons that show anomalies during routine surveillance of the stockpile. The high-temperature and high-pressure properties of what the Department of Energy calls key stockpile materials have already been studied. The results were then incorporated into simulations that have resolved, at least in part, the anomalous performance of devices tested many years ago.

The goal of the simulation program is to provide a tool for studying the behavior of older nuclear devices, perhaps showing the effects of corrosion, degradation of the high explosives or other composites, cracking, and other signs of aging. Simulation can also be used to study the behavior of nuclear weapons in abnormal environments, such as fire or plane crashes. Experiments using simulants to replace nuclear materials are permitted under the Comprehensive Test Ban Treaty (CTBT), but many more cases can be run at far lower cost on a computer than with hardware. This is a major benefit of simulation and ASCI, not only for the nuclear weapons community but also for other scientists and engineers. One need only think of the benefits of being able to simulate automobile crashes including every single part of the automobile on a computer with real accuracy.

The ASCI program is one of the most ambitious computer development projects ever undertaken. It will increase computer speed and capacity more than 50-fold in less than 6 years, beating Moore's Law which predicts the doubling of computational speed every 18 months for single processors by about a factor of 10. This is possible because the ASCI machines are massively parallel, being composed of up to several thousand individual computer processing unit chips. The fastest machine now available is the Lawrence Livermore National Laboratory (LLNL) *White* supercomputer, which has achieved a speed of 12.3 teraOPS. The ASCI *Q* computer will use nearly 12,000 processors and have a speed of 30 teraOPS when it is completed in 2002.

A major factor in the success to date of ASCI is the Academic Strategic Alliances Program (ASAP), which has brought the Nation's top supercomputer scientists to ASCI, leveraging their research to strengthen its programming efforts. This effort means that a great deal more manpower will be available for perfecting the techniques of large-scale modeling than if only weapons scientists were involved. The ASAP will also be an important factor in transferring the technology and techniques developed in ASCI to the private sector.

When the simulation tools have been properly validated, they should serve as the front-line method for understanding the implications of any anomalies observed in the stockpile. The results to date have shown that the program is on track and that it is already very capable.

A three-dimensional simulation of the explosion of a nuclear weapon primary was conducted on the IBM *Blue Pacific* supercomputer at LLNL in 1999. This computational experiment required the full machine for 20 days and used 300,000 megabytes of memory.[4] This first-ever three-dimensional simulation of a primary explosion revealed the cause of a mysterious test failure more than 20 years before.

structural performance and integrity of the earth penetrator bomb were simulated over a wide range of environmental parameters

Also in 1999, the ASCI *Red* supercomputer at Sandia National Laboratory completed simulations of a weapons system exposed to blast and radiation, correctly predicting the response of the weapon and providing tools to understand its vulnerability to a real nuclear battlefield environment.

Los Alamos, using the *Blue Mountain* supercomputer in April 2000, simulated the ignition and burn of a three-dimensional thermonuclear secondary. This program ran for more than a month and generated 15 terabytes of information. An exciting part of this simulation is that it was started on the *Blue Mountain* machine, ran for 820 hours, and then continued at the Sandia ASCI *Red* machine for 196 hours. This cross-platform result and the compatibility of the two very different machines goes a long way toward assuring that the ASCI program is producing reliable and error-tolerant code. The simulation included three-dimensional design features in the secondary and was compared to a nuclear test. An important step permitting high confidence in simulation was made when Los Alamos was able to run a three-dimensional computation of energy flow. This run took 18 days.

The structural performance and integrity of the B61 Mod 11 earth penetrator bomb were simulated on *Blue Mountain* in 23,000 separate runs to assess the reliability of the weapon over a wide range of environmental parameters. The resulting statistical analysis was validated against a small number of actual drop tests. Simulation permitted the designers of this new weapon to have high confidence in its performance and saved a significant amount of time and money by reducing the required number of destructive hardware tests.[5]

New Weapon Designs

For the 50-plus years of the nuclear age, it has been assumed that no nuclear weapon would be accepted for serial production and for inclusion in the U.S. stockpile without a full-scale test (aboveground before the Limited Test Ban Treaty of 1963, underground since then). One of the developments that permitted the United States to contemplate the total cessation of nuclear testing in the post-Cold War era was the seeming lack of any need for new weapon types or designs.

In the years since testing ended in 1992, the previous perception of many serving officers and national leaders that new weapons were unnecessary has begun to change. For example, C. Paul Robinson, director of the Sandia National Laboratory, has suggested the need to develop a low-yield earth-penetrating weapon that would enable the United States to hold at risk deeply buried command bunkers. A weapon of lower yield than the present earth penetrator, the B61 Mod 11, would be required to minimize collateral damage and fallout. Deeper penetration than can be achieved by the B61 Mod 11 would increase the coupling of energy to the ground, thus permitting the desired yield reduction. This probably would be an example of a new nuclear weapon that could be designed, certified, and produced entirely without a nuclear test, although most experts outside the Departments of Defense and Energy doubt whether fallout can be contained or adequate penetration achieved; those analysts also think low-yield weapons may be insufficient to destroy a hard and deeply buried target, and that any weapon with a yield that can destroy the target will necessarily produce a great deal of fallout.

Since the late 1960s, the United States has pursued one general type of nuclear weapon in many variants, ranging from low-yield battlefield weapons to high-yield designs suitable for attacking large areas or hard near-surface targets. Because the United States has studied this particular corner of design space in great detail for many years, it has significant information about which ideas work and which do not. The accuracy of new simulation computer programs can be tested against both this enormous database (comprising nearly 1,000 nuclear explosions) and the results of the legacy codes used to design the devices that were already tested.

Designs similar to those used for nuclear artillery shells should provide a baseline from which to produce plans for an earth-penetrating weapon in the low-kiloton yield range. An artillery-fired atomic projectile (AFAP) is subjected to roughly the same acceleration forces on launch as an earth-penetrating weapon is on impact. Consider the acceleration experienced by a 203-millimeter shell in a relatively conventional gun of 55 caliber[6] and a 900-meter-per-second muzzle velocity. If the force on the projectile is constant from firing until it leaves the gun,[7] then the average acceleration is 36,274 meters/second^2, or 3,700 times the force of gravity. Lateral vibration in the barrel is also likely to be severe but cannot be so simply estimated. If the same shell strikes the ground at its muzzle velocity (neglecting air resistance) and is so strongly constructed that it penetrates 10 meters into the earth before coming to a halt, the deceleration force on the projectile is almost exactly equal to that experienced during firing. In general, the deeper a munition is intended to penetrate the earth, the lower will be those decelerations because the weapon travels a longer distance before coming to rest.

Thus, existing AFAP designs are reasonable surrogates for the physics package needed in an earth penetrator. The performance of the earth-penetrating B61 Mod 11, which used a new case and an existing physics package, was computer simulated on machines considerably slower and less powerful than those available today.

If national decisionmakers commission a new earth-penetrating nuclear weapon, it should be possible to design and certify it without nuclear yield testing by using a procedure much like the following:

- Select an AFAP design comparable in size and yield to the military characteristics of the desired final weapon
- Modify the nuclear design in the smallest possible ways using ASCI simulation until the new weapon is considered able to withstand the decelerations expected on impact
- Design an appropriate case for the weapon, including whatever kind of penetrating nose is appropriate using the structural design codes made possible by the new generation of computers
- Test the implosion properties of the new primary (with simulants substituted for the nuclear materials) using existing or newer facilities, such as DAHRT, to ensure that the weapon functions properly before impact
- Drop test[8] an identical device in its casing; extract the physics package from the rubble; and then detonate the high explosives at DAHRT. The detonation system would not be live during the drop-test part of this experiment.
- After verifying that the physics package survives impact and performs properly, drop test another simulated device to verify that its high explosive detonates at the appropriate depth and velocity.

This procedure differs very little from what would be done if nuclear testing were allowed. Because the Limited Test Ban Treaty prohibits venting radioactive debris from a nuclear test to the atmosphere, a full-up test of the system would not be possible. The survival of a real physics package and its proper functioning after impact would, in any case, have to be inferred from the survival and functioning of a nonnuclear replica. In turn, the functioning of the replica would be checked at a hydrodynamic facility in the same way as suggested above.

General Considerations

Many of the difficult experiments involved in qualifying a new weapon based on an existing device design are nonnuclear and involve such issues as mechanical and electrical integrity and functioning after passing through a severe environment. Since none of these experiments would involve actual functioning nuclear components, they may be performed under all interpretations of the CTBT.

If new weapons designs are to be produced and certified without a nuclear test, they ought to resemble closely designs already tested. In particular, the shapes of the nuclear components and internal systems such as boost-gas piping, the type of high explosive used, and its geometry should be quite close to the tested designs, with the excursions well understood on the basis of both ASCI and legacy codes. Any new design should be conservative, not attempting to achieve reductions in size, amount of high explosive, and special materials. Additional plutonium or a different mixture of boost gas can convert a "prima donna" design into one that is more rugged and in which the designers can have more confidence.

An increase in plutonium or highly enriched uranium might reduce the safety margin of the device, while an increase in tritium in the boost gas could decrease the primary yield needed to initiate boosting. All of these tradeoffs seem possible, and the ASCI simulation capability gives designers their first opportunity to investigate the performance of a new weapon without first exploding it. Nevertheless, new weapon designs will likely resemble closely the designs of older weapons and come from the regions of design space where the United States has considerable experience, as they did when testing was allowed.

Notes

[1] *mega*OPS: million computer operations per second; *gigaOPS*: billion computer operations per second; *teraOPS*: trillions of computer operations per second. An *operation*, for example, is the addition of two numbers.

[2] *terabyte*: one trillion bytes. For comparison, the Department of Energy and others estimate that all the material in the Library of Congress together amounts to about one terabyte.

[3] *Mix* is the mixing of the inner lining of the hollow pit of a primary with the deuterium-tritium mixture, which causes boosting.

[4] For comparison, the computer on which this paper is being written is capable of several hundred megaOPS, has a 1 GHz clock speed, and contains 512 megabytes of random access memory, along with a 40 GByte hard drive. This is comparable to the capability of the Cray supercomputer on which the WB88 warhead was designed.

[5] Data on specific simulations taken from the unclassified fiscal year 2001 ASCI program plan, DOE/DP/ASCB2001BASCIBProgB001.

[6] *55 caliber* denotes that the length of the gun barrel is 55 times the diameter of the projectile, or in this case is 11.2 meters long.

[7] This is a reasonable assumption, although it is certainly not strictly true. However, it does provide a reliable figure for the average acceleration.

[8] Or, to achieve a higher impact velocity, one could accelerate the device electrically or with an attached rocket.

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