3-D codes yield unprecedented physics, engineering insights

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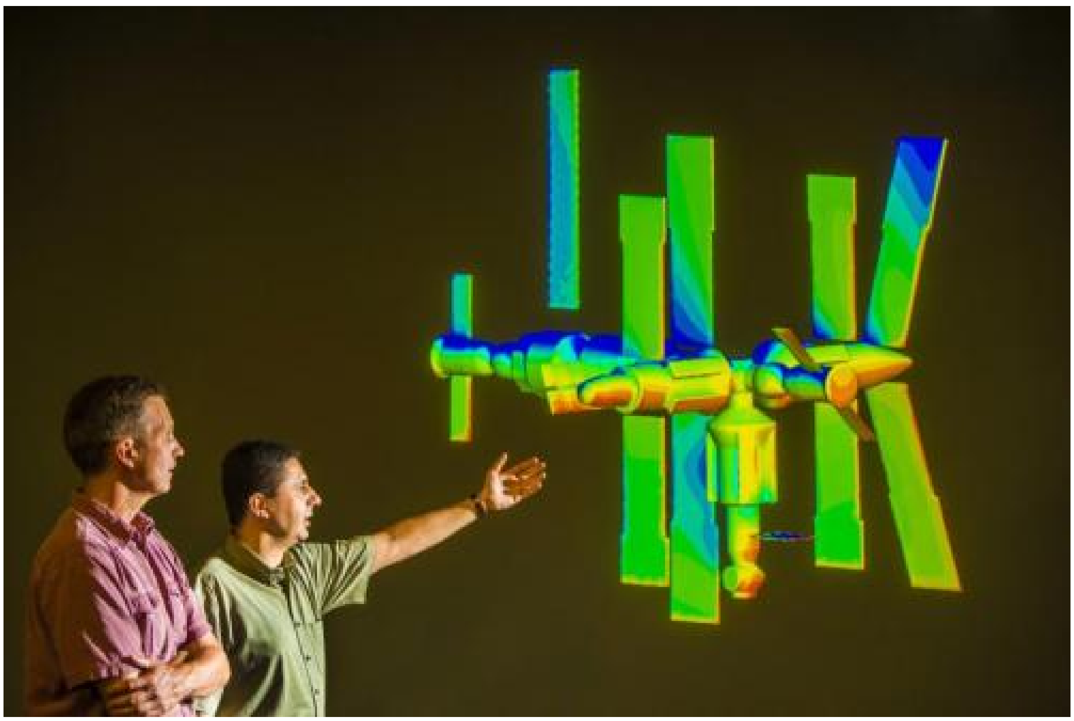

Sandia National Laboratories researchers Steve Plimpton, left, and Michael Gallis look at a projection of a model of the Russian MIR space station, which fell out of orbit several years ago and disintegrated, with the remains ending up at the bottom of the Indian Ocean. Using Sandia's 3-D code SPARTA, the calculation is simulating an instance of the process of de-orbiting. Randy Montoya

When the space shuttle Columbia disintegrated on re-entry in 2002, sophisticated computer models were key to determining what happened.

A piece of foam flew off at launch and hit a tile, damaging the leading edge of the shuttle wing and exposing the underlying structure. Temperatures soared to thousands of degrees as Columbia plunged toward Earth at 27 times the speed of sound, said Sandia fluid science and engineering researcher Michael Gallis, who used NASA codes and Icarus—a Sandia Direct Simulation Monte Carlo, or DSMC code—for accident simulations that proved critical to investigators.

The investigation helped researchers realize a more sophisticated code would be even more valuable in future inquiries at the same altitude and speed and for broader applications. Now Gallis and computational scientist Steve Plimpton have created a parallel three-dimensional DSMC code called SPARTA. In July, Sandia released it as open source, available to anyone here. In addition, Gallis presented results of work using SPARTA at an invited keynote lecture in China at the 29th annual International Conference on Rarefied Gas Dynamics.

Three-D codes like SPARTA represent physical reality more accurately than 2-D codes such as Icarus. Better simulations mean designers can account for many more details in new spacecraft or satellites. However, there's a computational price for greater realism. "A 3-D simulation is like a series of 2-D ones, sometimes making it thousands of times more demanding," Gallis said.

DSMC codes simulate molecules moving and bouncing off each other and objects, just as they do in real gas flows. Underlying statistics determine when and how molecular collisions occur, enabling predictions of energy transfer and chemical reactions. The DSMC approach typically is used to model low-pressure gases. Physical problems where gas is at low pressure are less common than problems with gas at higher pressures.

"Monte Carlo" refers to the randomized way in which collision parameters are chosen for pairs of particles, based on statistical principles. The order in which molecules collide is random, but not the rate or outcome of a large number of collisions, which can be described by well-known mathematical models.

Sandia recognized DSMC potential early

More than 20 years ago, Sandia researcher Tim Bartel and Plimpton developed Icarus, still considered a workhorse for DSMC applications. Gallis and Plimpton began working on SPARTA about two and a half years ago—doing some of their brainstorming while walking on the Santa Fe Plaza during breaks at an international DSMC workshop Sandia hosts every two years.

"Michael is very, very good with DSMC physics and Steve Plimpton is very, very good at formulating problems so that large parallel machines can solve them. That combination has given us a parallel code with very sound physics that runs quickly," manager Dan Rader said.

DSMC, invented in the 1960s by Graeme Bird when he was at the University of Sidney, takes a different approach from traditional codes that treat gases as a continuum rather than as individual molecules. Continuum codes solve partial differential equations based on such fundamentals as conservation of mass, momentum and energy. Although it's based on the same physical principles, DSMC's molecular approach lacked formal mathematical proof of its soundness until 1992.

"Until then, people assumed it was kind of an approximate method that could do the job in regimes where continuum methods would clearly fail," Gallis said.

Sandia is largely interested in DSMC for two research areas where gas molecules are relatively far apart: re-entry vehicles, including the effects of flight through the outer reaches of the atmosphere, and micro-electrical-mechanical systems (MEMS) that have features at the micron and submicron scale. Examples of MEMS include chemical flow and pressure sensors, accelerometers and transducers.

Senior manager Steve Kempka, who formerly managed one of the groups involved in the research, said the Gallis-Plimpton collaboration also has resulted in DSMC being used to simulate higher-density flows where molecules are relatively close to one another—something he never thought he'd see.

"DSMC will allow simulations free of the assumptions used in many other computational fluid dynamics methods. We hope it will let us explore the physics of turbulent flow in new ways. I believe we will see it being used to simulate re-entry vehicle flight to much greater depths in the atmosphere, with much more accurate descriptions of the flow," he said. That includes the difficult phenomena of laminar, or streamline, flow transitioning to turbulent flow; ionization of the atmosphere flowing around a re-entry vehicle; and the wearing away of material as a space vehicle races toward Earth.

The chaotic nature of turbulence makes it difficult to investigate, but Gallis said being able to use DSMC to study fluid mechanics at a more fundamental level may help to better understand the mechanisms of turbulence.

Parallel computing has broadened DSMC's uses

Particle methods like DSMC saw relatively limited use in the past, but parallel computing has broadened their applicability.

"We can now look at problems that years ago were unthinkable, or go well into the continuum regime, when we think the relevant physics needs modeling at the molecular level," Gallis said.

"Compared to Icarus, SPARTA enables us to resolve finer scales of behavior in low-density fluids and study flows around more complex geometries," Plimpton said. "In its development, we also thought about future, faster computers with novel architectures, trying to design the code to work well both on today's machines and tomorrow's."

With an open source code, Sandia is looking for collaborators to improve the code and enable users to add their own new physics, chemistry or collision models, Plimpton said.

"It's a win for Sandia because having additional developers expands the capabilities of a code more quickly and we get to use ideas that other people add to it and vice versa," he said. "It also introduces us to users who may discover coding errors or wish to collaborate with us on new applications."

The next frontier is to take advantage of DSMC to model and study flow physics—energy exchange and chemical reactions in colliding molecules—at a more fundamental level than possible with continuum codes, Gallis said. "If you're able to study things at that level, you are able to extract models that you can then use in continuum codes to study much bigger problems," he said.

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