

Leveraging ASCR Investments in Software Tools to the Broad Computational Community

Barriers to adoption of HPC modeling and simulation by the industrial computational science community can be tackled by getting DOE software in the hands of independent software vendors (ISVs) via SBIR/STTR

Opportunity

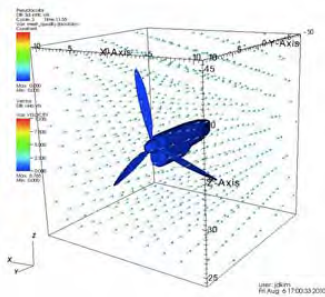
Over the past decade the Office of Advanced Scientific Computing Research (ASCR)* in the Office of Science has invested heavily in research and development of High Performance Computing (HPC) Software**. The DOE computational science community has embraced this software, which with minor steps is ready for adoption by commercial software vendors and industrial HPC users. As multi-core architectures and data challenges push industrial simulation to new heights, there is an opportunity to bring this HPC software, national laboratory expertise, and private sector computing challenges into closer collaboration. The integration and testing effort required to leverage this software in the private sector is within reach of modest sized programming and integration teams (1-5 people). In short, there is an opportunity to utilize this software for private sector simulation needs, albeit this software does not come delivered as a shrink-wrapped product.

As an example the Portable Extensible Toolkit for Scientific Computation (PETSc), is a suite of tools that form the building blocks needed to solve complex problems and deal with the massive amounts of data that arise in high performance computing applications. Although PETSc, a winner of a 2009 R&D 100 award, can simplify the process for solving these complex problems and has well proven

abilities it requires computational sophistication and expertise. In order to use PETSc, users may have to configure and build the package to suit their needs.

Another set of tools developed by the Applied Partial Differential Equations Center (APDEC) are applicable to problems in combustion, biology climate and other areas and can be used to simulate a broad range of complex physical systems. Many industries could use these tools but they also require efforts beyond those of commercial off-the-shelf (COTS) software. For these tools and the many others developed by ASCR to be accepted and used by a broader industrial computational community they have to be easier to install, troubleshoot and use.

According to recent studies conducted by the *Council on Competitiveness**** many industries can benefit from HPC, but there are barriers that inhibit its adoption. Two of the main barriers to adoption are: lack of application software, and lack of talent/expertise. Both of these barriers can be addressed by improving ways to get DOE developed software into the hands of software vendors who can then utilize their expertise to create and support production quality software for the broader HPC community. There is a great opportunity for software vendors to help bridge the gap between powerful ASCR software and industry.



Wind turbine generation simulation using FrontTier (image courtesy of ITAPS)



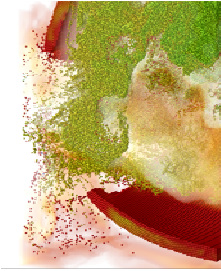
Smart Truck simulations helped to reduce fuel consumption by up to 12%

*<http://science.energy.gov/ascr>

**<http://outreach.scidac.gov/scidac-overview>

***<http://www.compete.org/hpc>

Challenge



Simulation of a rupturing steel container filled with plastic bonded explosive (image courtesy of VACET)

Despite the opportunity, ASCR faces many challenges in its efforts to promote industry adoption of tools and software it has developed. The main challenges are:

- Protecting intellectual property of ISVs
- ASCR's lack of experience in working with commercial software vendors and industrial HPC users
- Lack of priority for SciDAC Institutes* (cross cutting organizations funded by ASCR focused on computer science, uncertainty quantification and performance engineering research tools and software) to perform industry outreach
- No mechanism outside of SBIR/STTR to engage software vendors

Investment Strategy

- Create SBIR topics that focus on industrial outreach
- Take an active role in working with ASCR's research performers and facilities directors to find avenues to get ASCR software to a broader audience as well as leverage their industrial experience and contacts.
- Take an active role in meetings, focus groups, and panels that focus on industry adoption of HPC tools and services
- Organize workshops between industry, research communities and independent software vendors to focus on areas of collaboration
- Create an ad-hoc working group to coordinate efforts and make software available to the broader community:
 - SciDAC-3 Institutes
 - SciDAC Outreach Center
 - ASCR
 - Leadership Computing Facilities (LCFs)
 - NERSC
 - ESNET



Analysis of a temporally evolving turbulent jet flame (image courtesy of VACET)

Impact

- Creation of a direct pipeline for ASCR's software to software vendors
- Recognition of ASCR's efforts outside of the traditional science community
- Distribution of robust and powerful HPC software for no charge to US software vendors
- Adoption of HPC tools increased by the broader industrial audience
- Increased number of organizers eligible for INCITE
- Coordinated, real time SciDAC outreach and collaboration

FOR FURTHER INFORMATION CONTACT THE OFFICE OF
ADVANCED SCIENTIFIC COMPUTING RESEARCH
<http://science.energy.gov/ascr>

FOR FURTHER INFORMATION ON THE DEPARTMENT OF
ENERGY'S SBIR/STTR PROGRAM
<http://science.energy.gov/sbir>

*see: <http://science.energy.gov/ascr/research/scidac/scidac-institutes>