

From Algorithms to Applications: How Numerical Software Facilitates the Use of New Algorithms in Complex Science and Engineering Simulations

Carol S. Woodward*

* Center for Applied Scientific Computing (CASC)
Lawrence Livermore National Laboratory
Livermore, CA, 94550 United States
e-mail: woodward6@llnl.gov, web page: <https://people.llnl.gov/woodward6>

ABSTRACT

With continued advances in computing system capabilities, many scientific areas are simulating increasingly complex physical systems. These new complexities give rise to a demand for more accurate numerical methods that can handle these systems while running efficiently on high performance computing platforms. Along with these increases in simulation complexity there has also been a similar increase in simulation software complexity. As a result, there is a strong need for reusable, efficient numerical software that can incorporate algorithmic innovations from the applied mathematics community while facilitating high performance science and engineering simulations. In this talk, I will discuss advances in numerical software, high performance computing, and coupled model simulation and address how these advances connect to result in highly complex simulations. Examples from the application of the SUNDIALS suite of nonlinear and differential algebraic integrators to science problems will be included.

Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS- 869623.