The Flash Center

Educational Strategies in High-Performance Computing Simulations

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Educational Strategies in HPC Simulations

- Introduction
- Key Role Community Code Centers Can Play
- Importance of Educating Students in Verification and Validation
- Educating Students in HPC Simulations for Manufacturing
  - *A theme will be the importance and challenge of software development*
  - *A second theme will be the importance of the apprenticeship model of education and training*

Introduction

- I will address the questions given to the panel from the perspective of the Flash Center's experience in developing and using FLASH
- The FLASH code
  - Is a highly capable, modular and extensible, spatially adaptive hydrodynamics code that can simulate high-energy density physics and astrophysical phenomena (and even whole blood flow) that performs well on a broad range of advanced computer architectures
  - Has a built-in unit test framework that provides verifiability; this and a rigorous software maintenance process allow the code to operate simultaneously in production and development modes
  - Has a large community of users: it has been downloaded more than 1800 times, and has been used directly in more than 360 papers authored by more than 700 scientists
- The Flash Center has educated 29 Ph.D. students (2 were PECASE award winners and 2 were Krell Computational Science Graduate Fellowship winners) and trained 53 postdocs (24 are now faculty members at major universities) – 15 went to DOE labs

Importance of Federally Funded Research

- FLASH, and the educational and scientific achievements of the Flash Center, are the result of significant, long-term funding (lasting more than a decade) by the Academic Strategic Alliance Program of the ASC Program of the NNSA at DOE
- FLASH and the Flash Center are currently funded by DOE through the ASC Program in NNSA, and OASCR in the Office of Science; and by NSF through the Astronomy & Astrophysics Program, the Physics at the Information Frontier Program, and the PetaApps Program of the Office of Cyberinfrastructure
- The bottom line: federally funded research has been and continues to be crucial to the Flash Center's scientific simulations and its educational and training strategies

Key Role Community Code Centers Can Play

- The increasing importance of HPC simulations in science and manufacturing is a result of the rapid growth in computing power, and a parallel increase in the ability of computer codes to simulate complex phenomena
- This changing landscape increases the importance of community codes, and the centers needed to develop, use, and maintain them
- Curricula of most colleges and universities include courses in CS, solving PDEs numerically, etc., but little in the way of real simulations is present in classrooms
- Education and training in experimental science mostly happens outside the classroom through lab internships, summer jobs, the NSF REU program, graduate assistantships, etc.
- More education and training in HPC simulations could happen in this way – circumventing the often lengthy and difficult process of changing curricula

Key Role Community Code Centers Can Play

- Community code centers can play a key role in educating both undergraduate and graduate students in HPC simulations
  - Involve students in solving important, complex problems that only HPC simulations can address
  - Give students an appreciation of the crucial importance of having an interdisciplinary team that includes applied mathematicians, computer scientists, and application scientists in attacking complex problems through simulations, and allow them to be part of such a team
  - Instill necessity of professional coding standards and documentation
  - Instill need for codes to be subject to continuous, rigorous verification, including regression testing
  - Give students an appreciation of the crucial importance of validation
    - *These benefits extend to students outside the centers who use a community code in their research*

Importance of Educating Students in Verification and Validation

- Complex systems (e.g., astrophysical and high-energy-density physics phenomena, climate, airframes and aircraft turbine engines, smart grid, etc.) are ones for which an understanding of the behavior of the components in isolation does not suffice to understand the behavior of the system as a whole
- HPC simulations often are the only way to understand such tightly coupled, non-linear, multi-scale, multi-physics systems
- In such cases, establishing the degree to which the results of such simulations can be trusted is vital, particularly when (as is increasingly the case) major business and governmental decisions are based on them
- Verification and validation (V&V) of HPC simulations have therefore become vital
- Given this, it is essential that students gain an appreciation of the crucial importance of V&V and learn how to do it, but in many fields this is not happening

Importance of Educating Students in Verification and Validation

- Also, the current methodological approach to simulating complex systems is usually to identify key sub-systems or processes, understand these in isolation, and then consider the full, re-assembled system
- But such an approach may not uncover all of the important sub-systems or processes, nor does it necessarily provide guidance about how to do the re-assembly
- Current methodological approach to V&V ("hierarchical V&V") mirrors this approach, and therefore has similar limitations
- Students need to be educated to explore new methodological approaches to both simulations and V&V
- Possible educational strategies employing the apprenticeship model include
  - Leveraging community code centers (as discussed above)
  - Fellowships and internships focused on V&V at national labs
  - Fellowships and internships focused on V&V at OEMs

Strategies for Educating Students in HPC Simulations for Manufacturing

- In an increasingly globalized world, U.S. manufacturers must compete on innovation, not cost
- Greater use of HPC simulations by U.S. manufacturers is critical to innovation
- The Council on Competitiveness formed a Working Group on HPC and Manufacturing ~ 2 years ago to identify the structural barriers and obstacles that are preventing this, and propose solutions
- The failure of the U.S. to create state-of-the-art codes for manufacturing and to support SMEs in adopting them are key issues identified by the CoC Working Group
- A possible strategy is creation of HPC and Manufacturing Service Centers in each of the 50 states – analogous to the agricultural extension service – that would help to achieve both

Strategies for Educating Students in HPC Simulations for Manufacturing

- A third key issue is the failure of the U.S. to educate and train young scientists and engineers to exploit HPC simulations for manufacturing
- A possible educational strategy is a public-private partnership
  - Federal agencies should consider creating fellowships to train undergraduate and graduate students in HPC simulations for manufacturing
  - PECASE could be expanded to include awards in HPC simulations for manufacturing
  - OEMs could create matching fellowships and internships
  - All these programs could be linked through the HPC and Manufacturing Service Centers to internships and summer programs at OEMs and at SMEs that already use or want to start using HPC simulations