Role of computational science in accelerating scientific discoveries and technology innovations for sustainable transportation

Sreekanth Pannala, Oak Ridge National Laboratory
pannalas@ornl.gov

Today, making gains in vehicle efficiencies is becoming extremely difficult as one needs to consider the complex interaction between the engine, battery, power electronics, materials, controls, aerodynamics, etc. and find optimal solutions that provide safe and affordable vehicles with small carbon footprint. It is thus important to codify and automate the knowledge and intuition we have collectively acquired so far and use our precious human resource for the creative solutions that build upon that. Computational science is prime to tackle this challenge as it is the only tool within our reach to get an handle on the exponential increase in the vehicle calibration space that is needed to find optimal designs. Computational Science, the field of using computers and numerical algorithms/methods to enable scientific discoveries and technology innovations, is a rapidly growing field that has a huge potential to revolutionize the way science and engineering has been performed for centuries. For this reason, it is often called the third pillar of modern science complimenting observations and theory. Since the advent of transistor (not so long ago) and rapid innovations in the electronics industry, the computing power has increased exponentially with extreme affordability (the GPU on Ipad3 has 32,000 X operations compared to mainframe from the 60s). The modern supercomputers utilize large number of such compute cores (100s to millions) to provide compute capabilities that we did not even dream off few decades back. It is the challenge, great opportunity, and promise in front of us to translate the knowledge we have acquired through observations and adapt the existing theoretical frameworks to generate clear set of instructions that we can compute at scale to simulate real-world applications. The integration of observations (through advanced characterization), theory, computations, and now data would be the driving force of science and technology for sustainable transportation but also broader field of management of energy and water resources while minimizing environmental impact. In this talk, I will give specific examples of computational effort related to transportation (engines, battery performance and safety, pyrolysis of biomass for transportation fuels, thermal management in power electronics, etc.) and lay down a roadmap as to how we can utilize HPC to accelerate the design of highly efficient and cost-effective vehicles that meet the regulatory, safety, and consumer demands going forward.