Evening Meeting Topic

Task: Describe your discipline's scientific goals the require further investment in HPCD resources and service in one sentence that is understanding and motivating to the general scientifically supportive public.

In ten years, we will be able to predict the molecular mechanisms for protein conformational changes on the time and space scales observable via light microscopy.

For moderately sized bio-molecular (riboswitch, enzyme) will be bale to fully elucidate the conformational ensemble and assess/calibrate experimental interpretations.

Starting at the initial fluctuations from the Big Bang, we will be able to model the shapes and sizes of galaxies in all environments done the smallest scales observable.

The synthesis of lattice QCD calculations and new experimental results from the Large Hadron Collider will shed light on physics that lies beyond the standard model of particle physics and the Higgs Boson.

Emergency management will be able to take advantage of geospatial big data, cyberGIS analytics and high spectrum computing for achieving scalable planning, preparedness and response.

With Exascale computers, scientists will be able to finally rain formation reliability taking into account small scale turbulence, phase change, thermodynamics and atmospheric science. This will be a breakthrough highly relevant to predication of the effects of hurricanes.

Without advanced computing, experimentalists and modelers in turbulence will not be able to validate their results and design of practical engineering devices will suffer accordingly.

In five years it will be possible to have adaptive, scalable software that enables computer engineering to be computed on computers with capabilities of running at 100-200 Petaflops.

In ten years, lattice QCD calculations will increase in precision from 1% to 0.1% to match the precision of particle physics experiments searching from evidence of physics beyond the standard model.

Understanding the function of proteins by being able to simulate them with atomic resolution for realistic time scales (3-4 orders of magnitude longer than achievable today) leads to a fundamental understanding of their malfunction in various diseases.

A major goal is computation nuclear physics is to understand from first principles the fusion of 3 alpha-particles to from carbon; a key process in the formation of elements (nucleosynthesis).

Climate: Where does the science need to be for computing in 5 to 10 years

Over the next 5 years, the focus will be getting very high resolution models ready and running for the next major international climate model intercomparison CMIP6, which will likely produce 5-10 PB of data for analysis. The analyses of past, present, and future projections of climate from CMIP6 will provide important input into the next IPCC and NCA assessments as well as contribute extensively to impacts and policy related analyses. Our aim for CMIP6 is to have some global models run at as high a resolution as 1/4° (25 km resolution).

Over the next 10 years, we will be aiming for even higher resolution, perhaps more like 4-10 km models that are cloud-resolving. Although improvements in the representation of physical, chemical, and biological processes in the models are also important, high-resolution simulations are imperative because of the enhanced, detailed information they can give through better representation of orography and local processes, and resulting effects on synoptic scale weather structures across the planet.

The primary science goal of gravitational wave physics in the next 5 years is the detection of gravitational waves and the beginning of observational gravitational wave astronomy with the advanced LIGO instrument.

In the next 5 years, we aim to carry out enough long, accurate full general relativistic simulations of black hole/black hole and neutron star/black hole binaries to provide wave forms to test GR via LIGO observations to the full accuracy of the instrument. In the next 10 years, a key goal is to carry out GR + relativistic MHD + neutrino transport simulations with enough accuracy and enough physics to solve the supernova mechanism problems, as well as nucleo-synthesis from neutron stare binary mergers.

In the next 5 years, the space physics community should expect hybrid, multi-scale numerical models capable of combining an MHD approach globally while solving the kinetic Boltzmann equations locally, which will need exascale supercomputers and Petascale data files. Solving the Boltzmann equations directly will require 6-dimensional parallelization strategies and innovative data-handling technologies.

Solve the quantum mechanical few body problem.

I would like to see all science codes running at >25% of peak of the limiting resource (scalar/parallel Flops, memory BW, interconnect, etc.)

Possibly make a material or device design insight to keep Moore's law alive.

Do a totally ab-initio calculation of the simplest high-temperature superconductor and make comparisons with experiments, which would service as a landmark in materials genome (discovery by predictive computing)

Supercomputing will enable climate scientists to make accurate enough predictions to improve agricultural practices to enable the earth to sustain all people on it.

Advances in high-spectrum computing are needed to improve our understand in everyday physical phenomena, such as turbulence, to improve our ability to applied science for the good of mankind.