

Numerical Laboratories in Exascale Simulations

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World-wide there is an ongoing effort to build an Exascale computer. Such a machine will enable simulations of physical systems at unprecedented detail. Some of the largest particle-based simulations today (like those in cosmology) already exceed a trillion particles. Exascale simulations will have much higher resolution, with memory footprints in several petabytes. As a result, in the Exascale world only a small fraction of the complete output can ever be saved for later reuse and much of the analysis will have to be done *in-situ*. At the same time, as fewer and fewer researchers will be able to directly access these ever larger systems, it will become increasingly important that data products from the largest simulations be released, shared, reanalyzed and archived over extended periods by the broader science community.

Scientists in many disciplines would like to compare the results of their experiments to data emerging from numerical simulations based on first principles. This requires not only that we can run sophisticated simulations and models, but that at least a selected subset of the results of these simulations are available publicly, through an easy-to-use portal. *We have to turn the simulations into open numerical laboratories in which anyone can perform their own experiments.*

We propose to put forward an idea, based on an analogy from particle physics, namely the LHC experiment. At CERN the particle collider has multiple “*beamlines*” that host enormous particle detectors. These instruments detect collisions at such a rate that the physicists use hardware triggers (essentially *in-situ* processing) to eliminate most of the data, keeping only 1 in 10 million events with the highest likelihood to lead to new physics. This small fraction of the data is still about 10PB/year, keeping the whole particle physics community busy for years. This difficult tradeoff was reached over a very careful evaluation of the different conflicting factors, like event rate, storage budget, etc. There is an important lesson to be learned from this example.

Once simulations take many billions of CPU hours, combined with a small number of Exascale machines, individual groups will no longer be able to run their own separate simulations. Instead, most likely a wider community will have to join forces to attack a particular problem, share the simulation, but provide their separate “detectors”, plug-in operators, similar to the LHC beamlines. These operators can analyze and, if necessary, save smaller subsets of the data in secondary storage. Their execution will be fired by *in-situ triggers*, reacting to particular patterns in the simulation, possibly based on machine learning algorithms. These smaller subsets of all the interesting events can then be shared by the broad community.

These software components together can be thought of as “*immersive virtual sensors*” and can either provide a one-time measurement, or a continuous stream of data (at a possibly high temporal resolution) from a neighborhood around a given location. The sensors can stay at a fixed location, or they can move with the flow. They can react to extreme events, but also sample the background field at statistically meaningful locations, to provide a reference for the overall system behavior. If there is a way to store a few previous snapshots in burst buffers near the CPUs, one can also save limited “precursors” of the triggered event streams.

Such a *hitchhiker pattern* presents a transformative change in the way we view simulations in general. Currently most simulations are thought of as a sequence of “static” snapshots, saved at time intervals large w.r.t. the time resolution of the simulation itself. We posit that instead one should see them as a massively parallel set of temporal streams, where each Lagrangian particle can be followed along its trajectory, or each region of interest (halo, vortex tube) can be tracked; and all of it happening at the high temporal resolution of the simulation.