Using Paraview® on subMIT for 3D Visualizations

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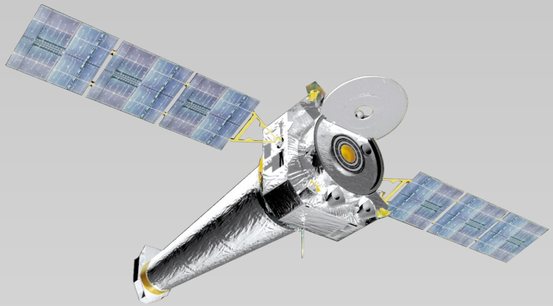
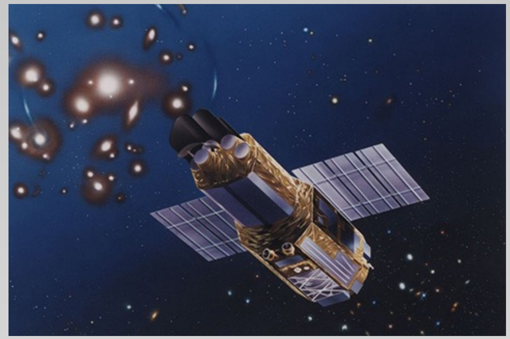
A Little Background

- **Our group is primarily involved with the design, fabrication, deployment and operation of x-ray photon detection instrumentation used for space based soft X-Ray Astronomy in the 0.2 – 10 KeV range**
- **A subset of our interests is the modeling of detector responses due to such things as initial design parameters of the detector and environmental effects on detector performance**
  - *Many of our past and proposed future missions involve the design and fabrication of custom-made detectors in close collaboration with MIT-LL Microelectronics Group, who have their own silicon foundry facilities on site*
  - *There are many knobs to turn and parameters to tweak to optimize the sensor for a specific mission's requirements*
- **Most of the modeling and analysis can be done utilizing standard computer workstation class computers. However, there are a couple of cases where HPC resources have been leveraged to make the simulation feasible**
- **The first HPC project we embarked on was in conjunction with the European Space Agency's Athena Mission's Wide Field Imager (WFI) Project to study** *Background Variability due to Galactic Cosmic Rays*
  - *Generate a GEANT4 based model of the WFI instrument and subject it to Galactic Cosmic Ray (GCR) spectra to model the in band unrejected background*
  - *Use this information to help understand the background variability, based on GCR variability*
  - *A side project we have with a group at Stanford, is to provide them with simulated GCR effected frames where they try to train various AI tools to help identify unrejected in band background signal*
  - *While we initially built the model on a workstation, we ported it to an HPC cluster (in this case Supercloud) in order to to ramp up the GCR particle count, to the >1G primary particle per run range*
- **The second HPC project build a** ***Poisson Solver Model*** **of a segment of a CCD imaging area** ***to model electron drift/diffusion*****, due to the imposed electric field impressed across the detector, of the photoelectrically generated electron cloud from the initial x-ray interaction point to the buried channel for readout. This was a natural follow-on to the Geant4 WFI Project. This model was also ported to MIT-LL Supercloud**
- **Both projects produce very large datasets in the Giga to Terabyte ranges which needs to be analyzed and would benefit from some advanced 3D Visualization, This is where Paraview on SubMIT came in**

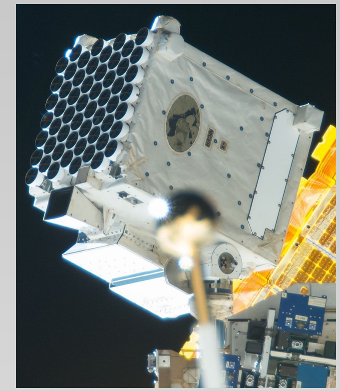
Backup Picts



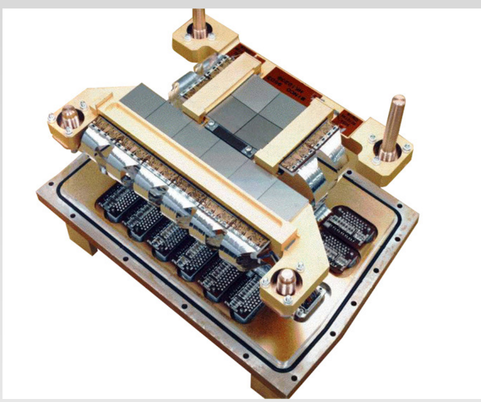
Chandra X-Ray Observatory



Suzaku X-Ray Observatory

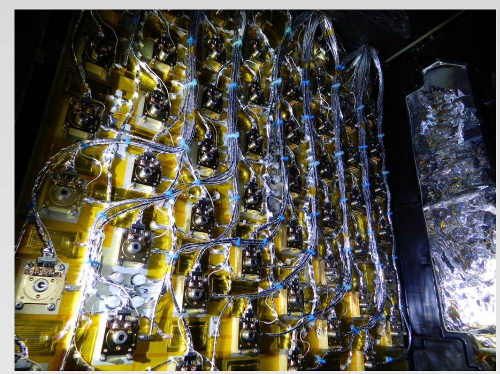


N**eutron Star **I**nterior **C**omposition **E**xplore**R



***A**dvanced **C**CCD **I**maging **S**pectrometer*

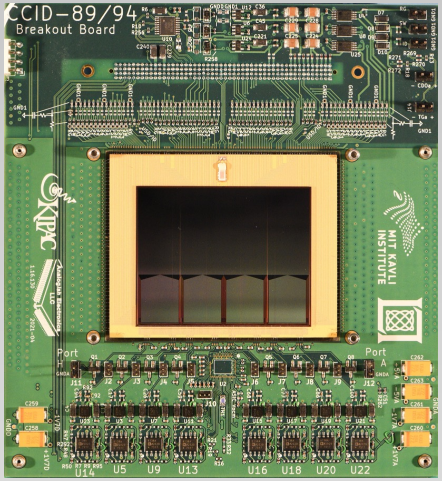
***X**ray **I**maging **S**pectrometer*

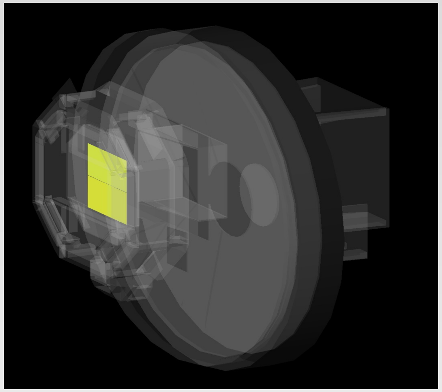


Nicer Focal Plane

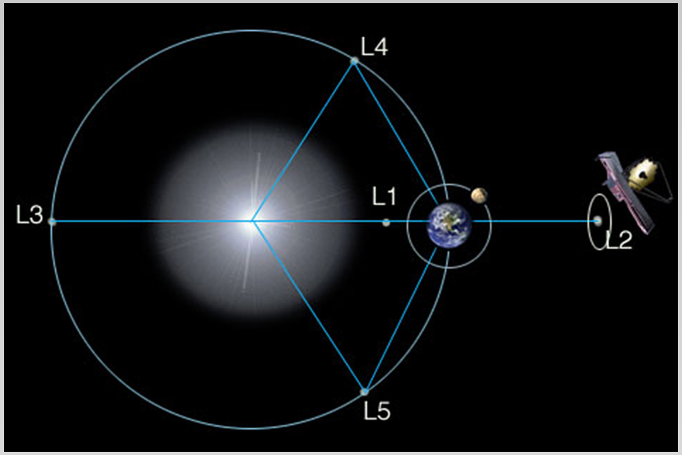
Detector Background Energy Deposits Modeling using Geant4 Toolkit

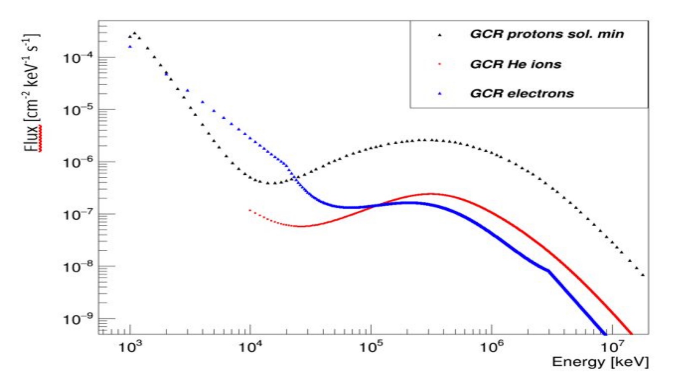
Instrument Hardware



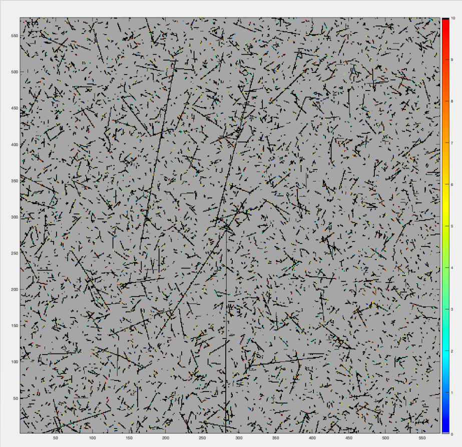


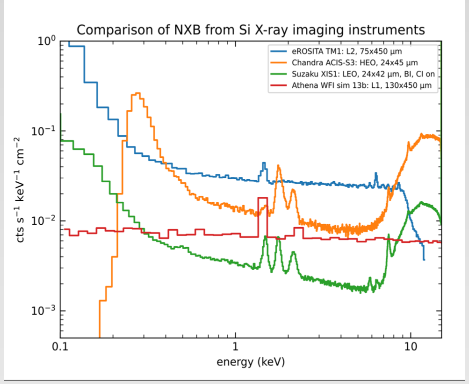
Radiation Environment





Energy Deposits





Example HPC Resource Requirements

3×10^9 Primary GCR Protons

24 Nodes with 48cores/node ***=1152cpus*** on MIT-LL Supercloud

Run Time: **~20 hrs for Geant4 and 3.5 hrs for post-processing**

Log Files: **> 1.5Tbytes**

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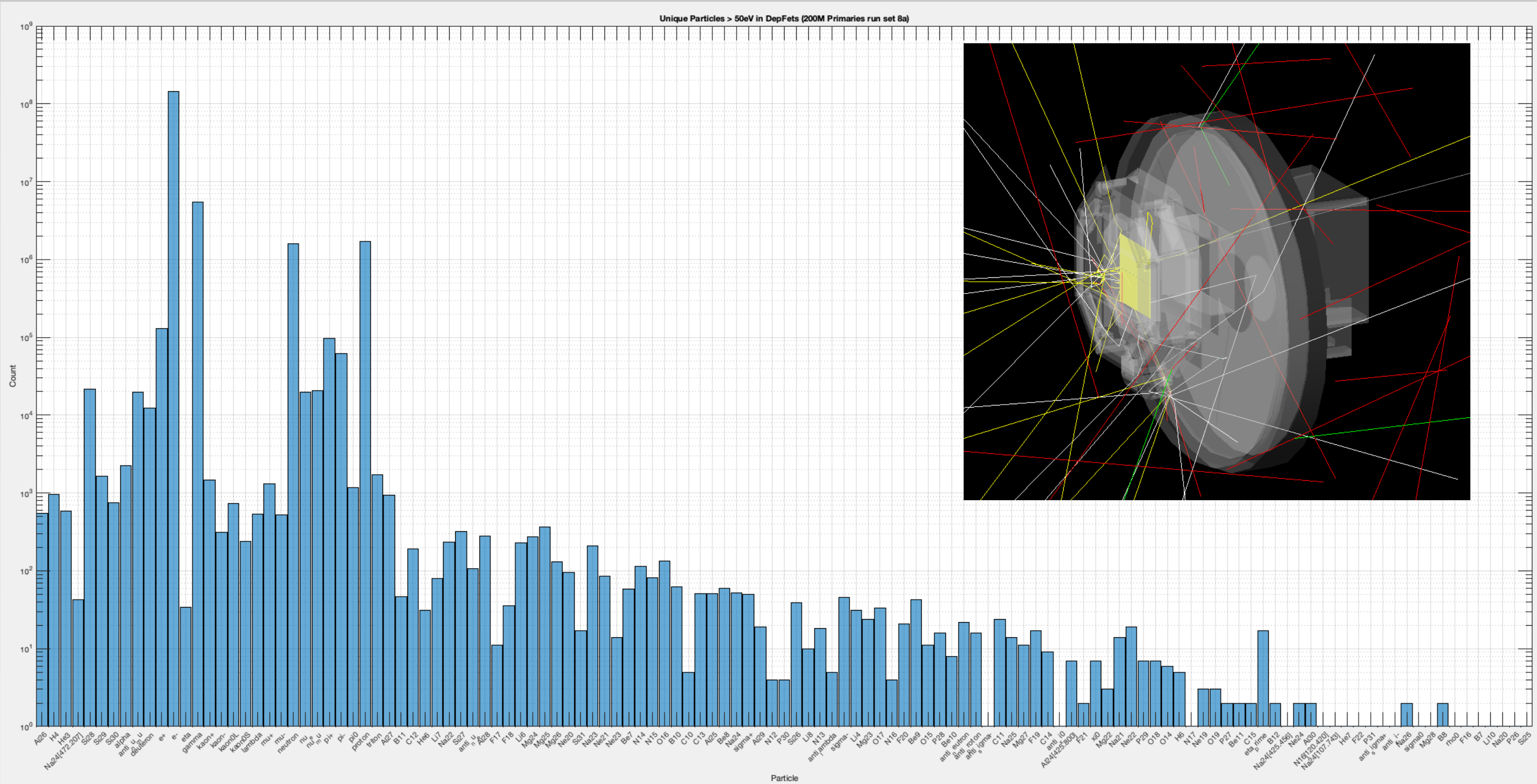
Backup Picts



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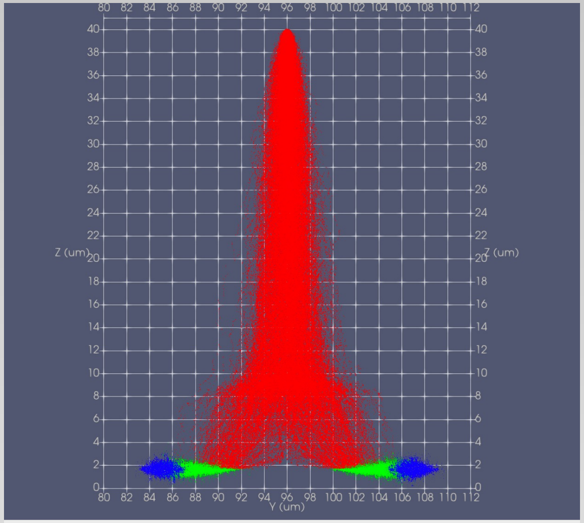
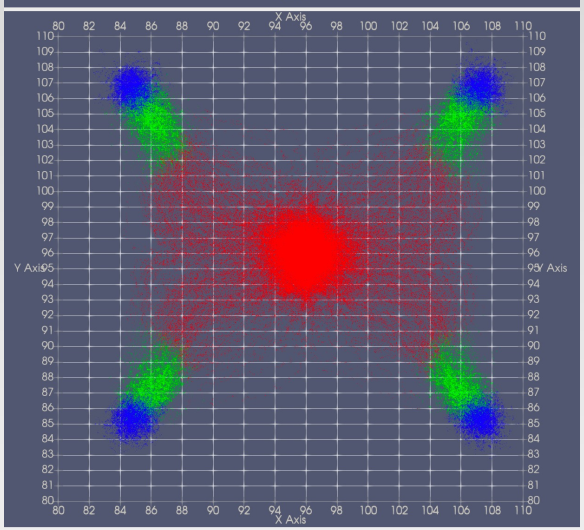
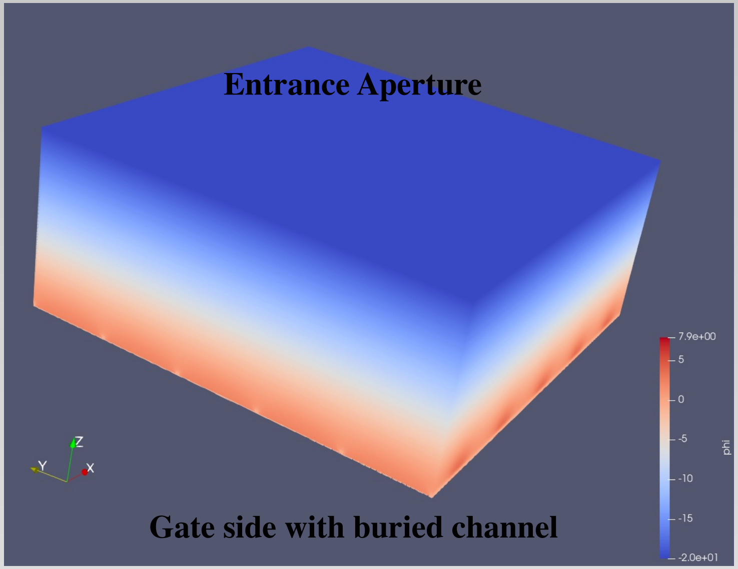
Poisson Solver Project

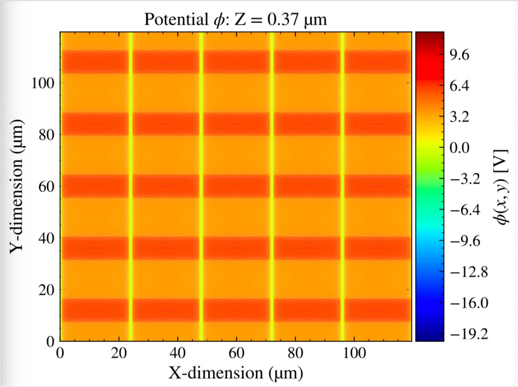
- **The previously described Geant4 GCR project, mapped the resulting energy deposits, in electron volts (eV) from various physics processes to XYZ locations within the Imaging Area of the detector**
- **Depending on the process associated with each particle step, those energy deposits need to be converted to electron-hole pairs**
  - *An instrument specified to cover the soft X-ray band from 200eV to 10KeV band will produce electron clouds in the 55e$^-$ to 2740e$^-$ range*
- **The internal electric fields (both static and dynamic) imposed on the detector, along with some other design features of the detector, will determine how those electrons drift/diffuse through the detector from the interaction point to the device buried channel where it is subsequently transferred to an output node for digitization**
- **Modeling of how that charge cloud diffuses is an important step in determining how the charge will be split between neighboring pixels, which has an important effect of the final energy resolution of the detector**
- **Just the matrix used to hold the solved electric potential grid of a small detector subarray of say 5x5 pixel x 50um thick can be large**
  - *300 x 300 x 600 = 54M double values, so memory requirements are modest by HPC standards*
- **Doing the electron Monte Carlo propagation thru the subarray is compute intensive. A Single X-Ray can generate up to thousands of electrons, which need to propagate hundreds of steps and tens of thousands of X-rays are needed to be simulated for decent statistics.**
- **Our next step is to try to develop an analytical approach to predict the charge redistribution from the initial interaction site to the final pixel accumulation sites, thus significantly reducing the CPU resources needed to do the Monte Carlo simulation for each photon.**

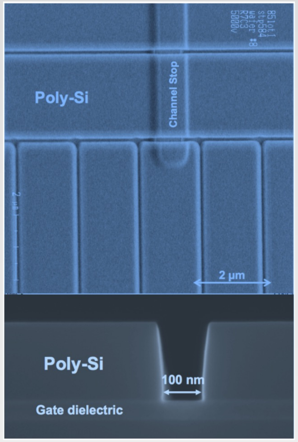
Backup Picts





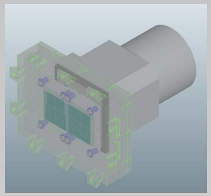


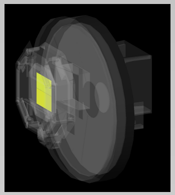


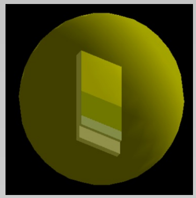


Review of General Processing Flow

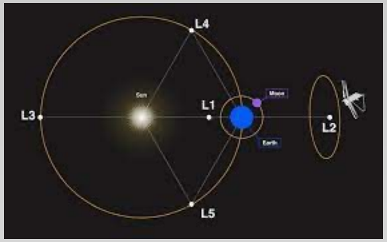
Build a Geant4 based model of a Silicon Detector nested inside its housing.
(CAD/Geant4)

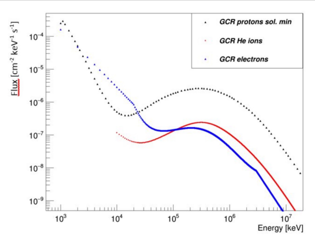




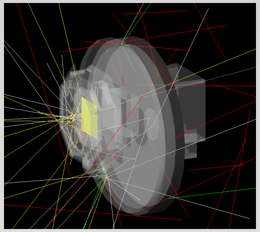


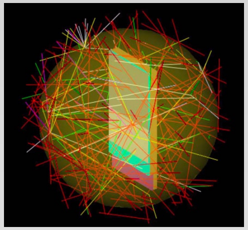
Immerse that Instrument in the expected radiation environments, such as the Galactic Cosmic Ray environment at the Lagrangian Point 2 (L2) Orbit for the Athena WFI Instrument
(Geant4)

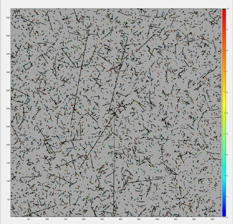




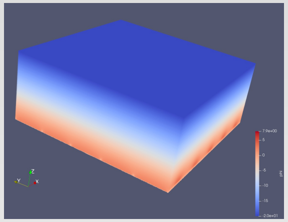
Track all the 3D energy deposits from the primary and secondary particles traversing into/thru the Imaging Area of the detector, converting those energy deposits to electron/hole pairs in the depleted region of the imaging area of the detector
(Geant4 & Python Post Processing)

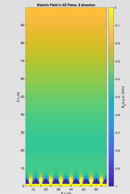




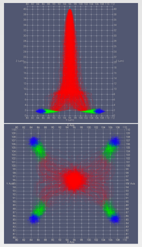


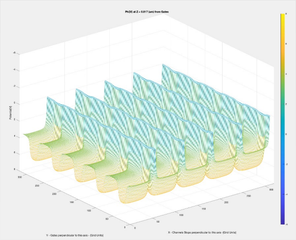
Model the EM Internal fields of the Silicon Detector Imaging Area in order to transfer the electrons (Subject to drift and diffusion) from the deposited energy interaction sites to the buried channel
(Poisson Solver)

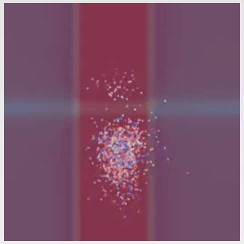




Analyze Data, which includes providing 3D Visualizations of the electron tracks and the internal field structure of the Detector Imaging Area
(Paraview)







Large Data Visualization using Paraview

- **Both Cluster based models (Geant4 and Poisson Solver) can produce copious amounts of data products (typically in the Giga to Terabyte range)**
- **Much of this data can be reduced to simple forms (descriptive statistics, histograms, correlation matrices, etc)**
- **Some visualization can be done easily on a workstation using common tools (Matlab, IDL, pyplot)**
- **More complicated mixed dataset 3D plots can benefit from a visualization tool that is designed to process very large datasets and can run on an HPC cluster where the data resides, making use of its available resource such as GPUs, large shared memory, multiple cores, etc**
- **Pretty straight forward to install Paraview on SubMIT**
  - *We could have tried this also on MIT-LL Supercloud but wanted to take SubMIT for a test drive*
  - *Available as source code or binaries*
  - *Did not need anything like Docker or Singularity*
  - *Client-Server operation between Workstation and Cluster worked well, once SSH tunnelling was set up between workstation, in our case a MacPro, and the SubMIT compute node*
    - Kudos to Matt Heine for figuring it out
- **All in all, Paraview takes a little getting used to. It might not always seem intuitive and if you do something wrong, it can go out to lunch on you**
  - *Well, after all is is open-source community software*
  - *There is a user group where you might get some help, along with some You Tube videos*
  - *Documentation is not all that great, but typical of modern programs and APIs.*
  - *I have a very low threshold for computer induced pain and was still able to get things going, producing some useful visualizations*

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Paraview GUI Interface looking at simple static electron track points

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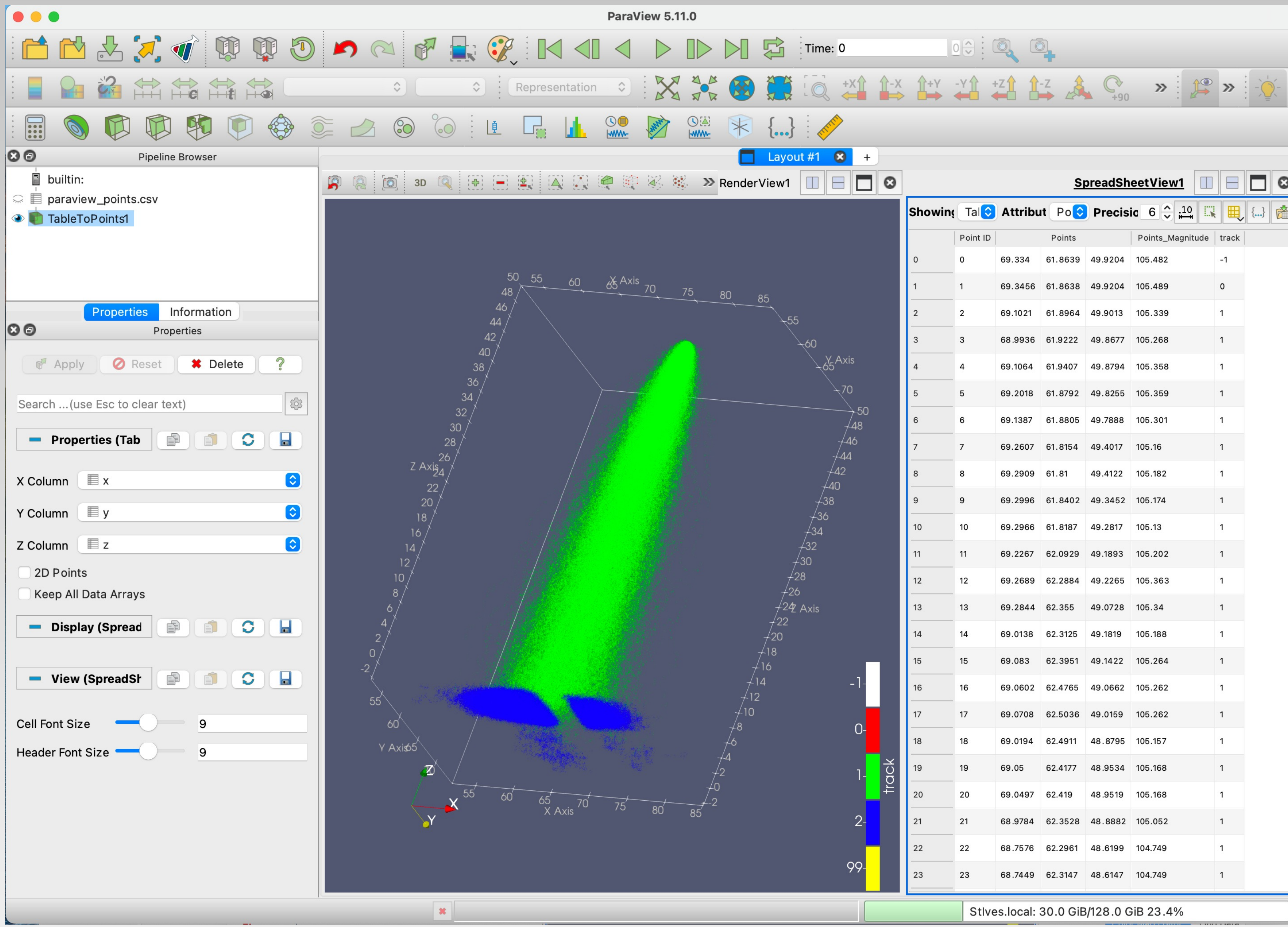
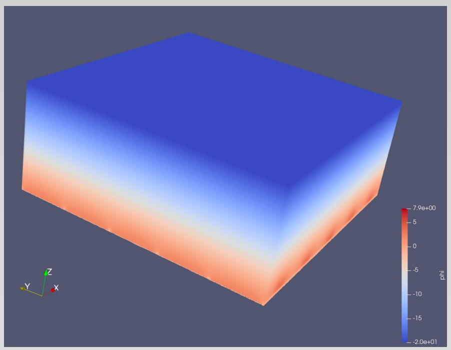
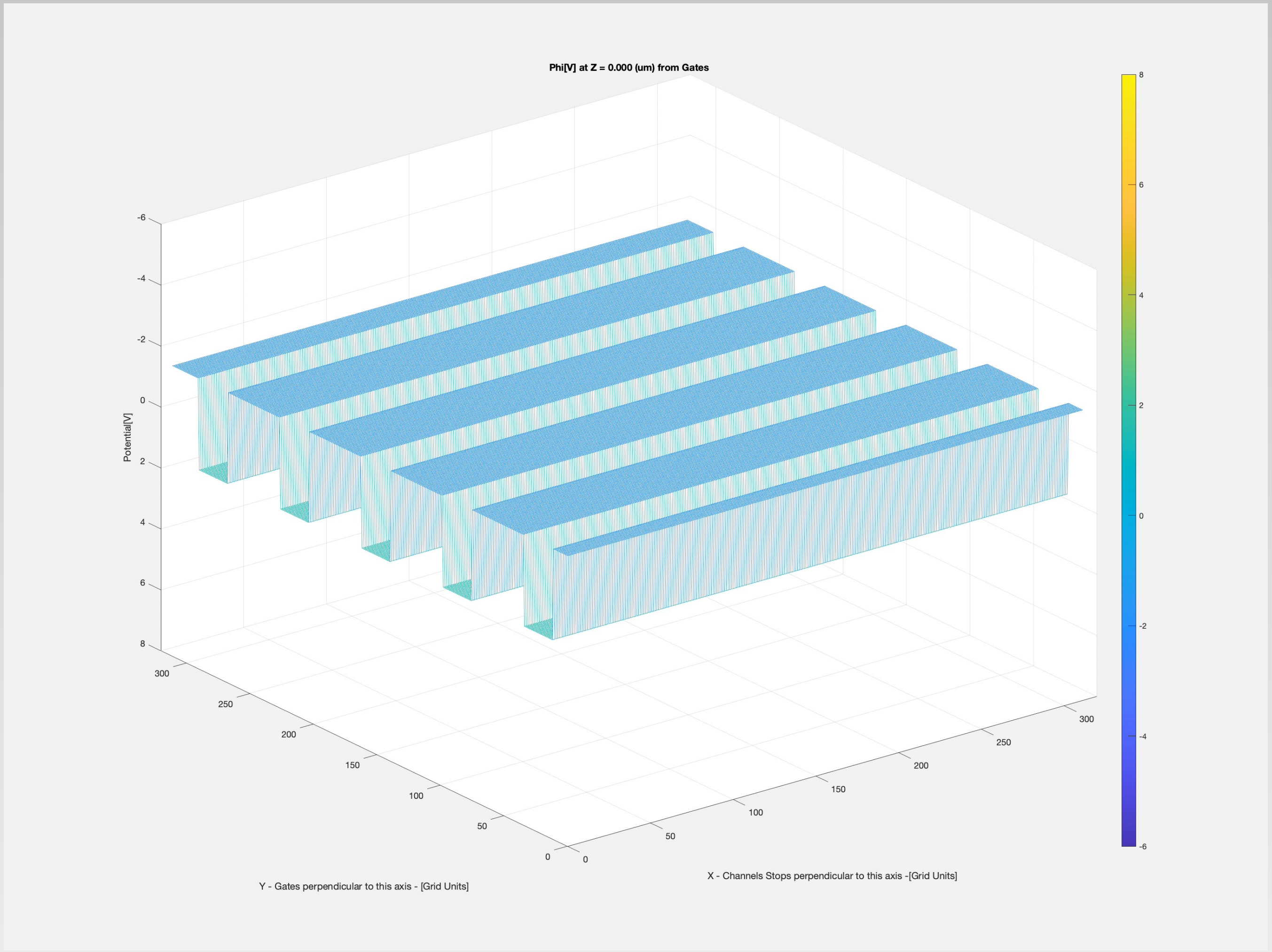
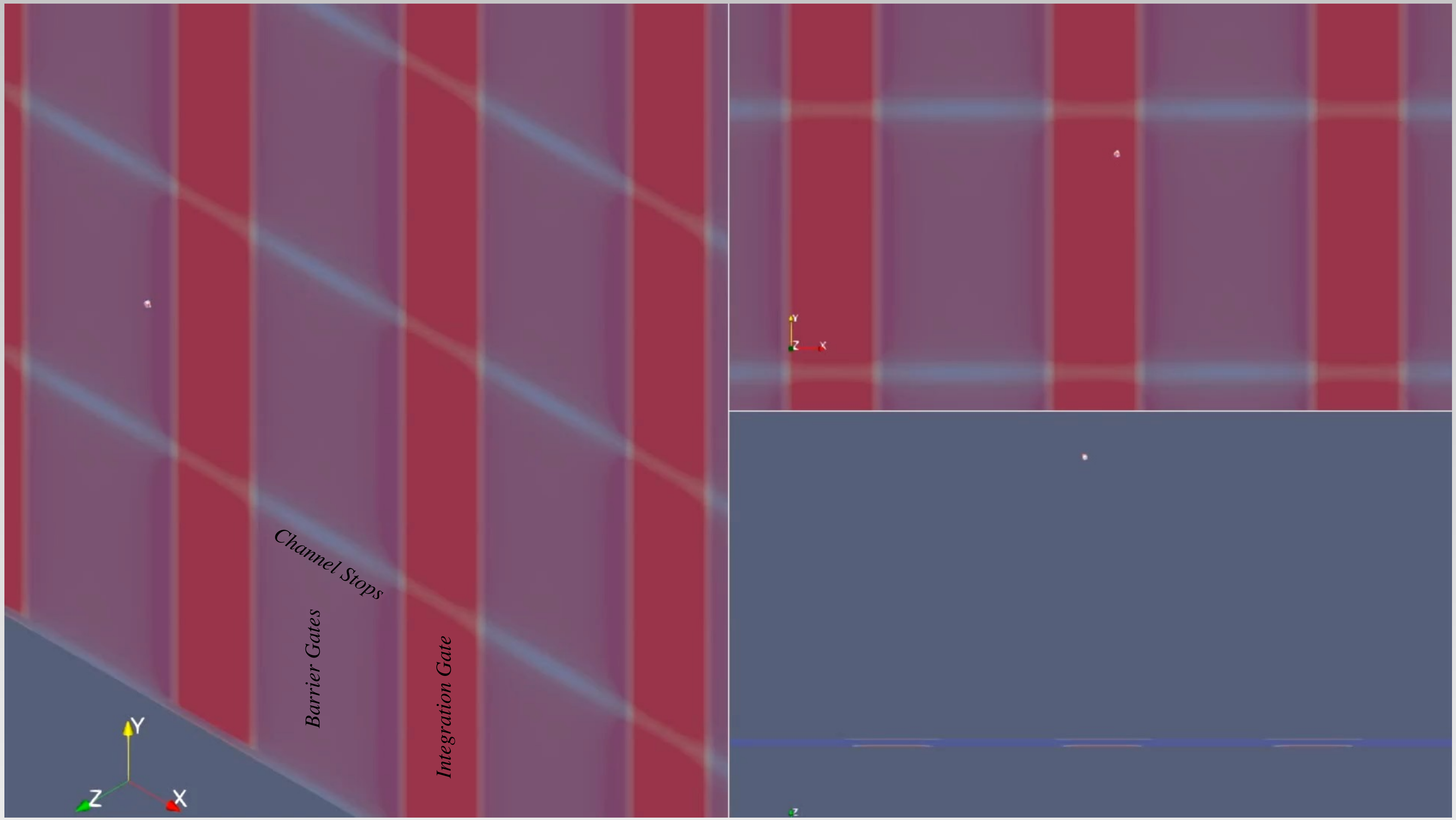


Potential Map Scan from Imaging Area Gates towards Entrance Aperture





Merging Potential Map Slice with Time lapsed Particle Tracks in 3D



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Paraview Highlights

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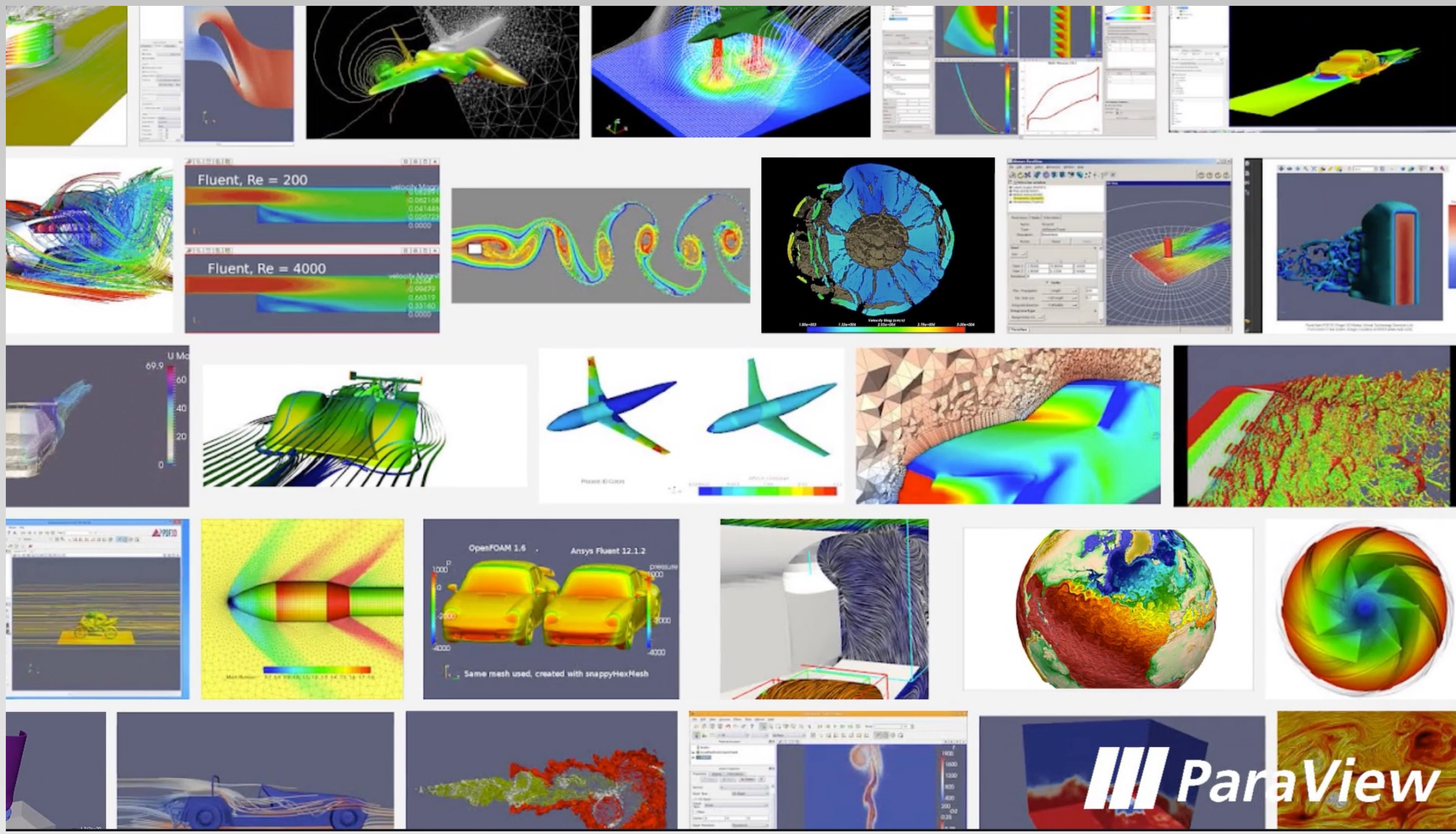

Los Alamos National Labs roots | **Open Source/ Multiplatform** | **Scalable: Workstation to HPC Environments**

GUI Interface/Python Scriptable | **Specializes in Large Datasets** | **Client Server Model: Desktop and HPC Cluster**

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https://www.paraview.org/

Paraview overview

ParaView