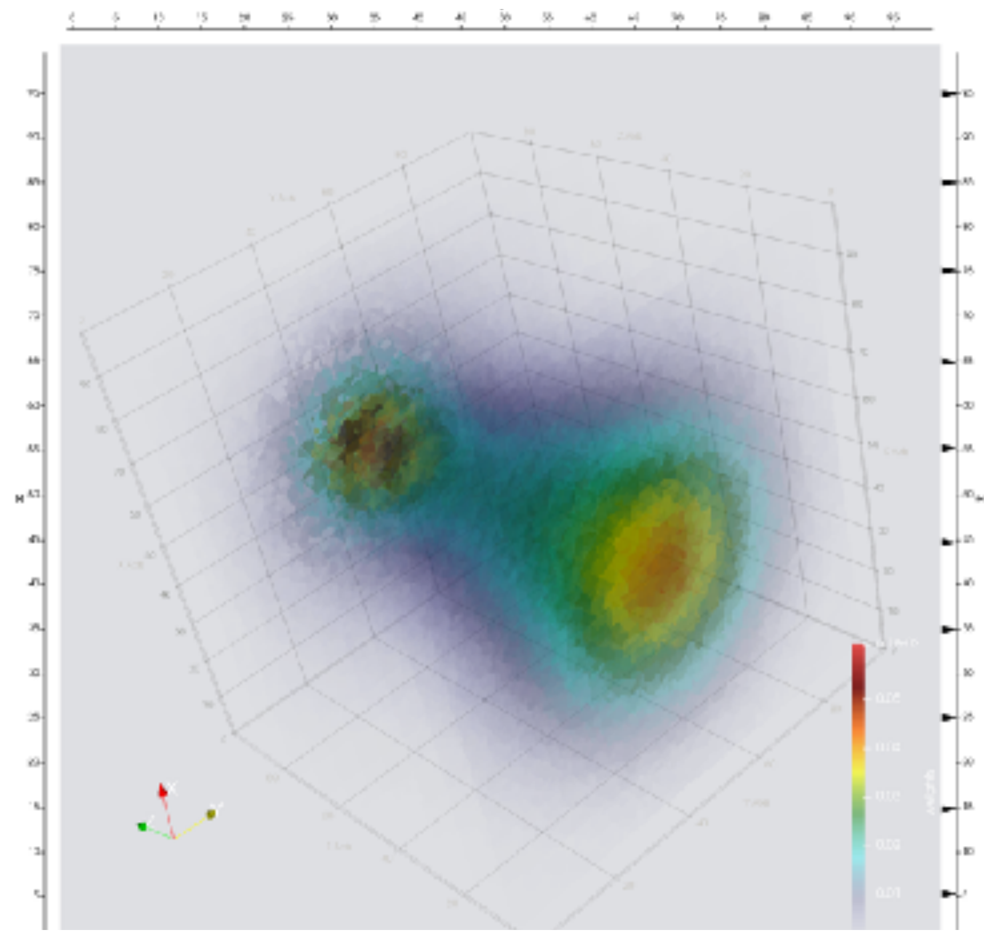
Next-Generation Imaging Filters and Mesh-Based Data Representation for Phase-Space Calculations in Nuclear Femtography (CNF19-04)



Gagik Gavalian (Jefferson Lab)
Nikos Chrisochoides (ODU)
Christian Weiss (Jefferson Lab)
Pawel Sznajder (NCBJ Warsaw)
Christos Tsolakis (ODU),
Angelos Angelopoulos (ODU)

The work at ODU (CRTC) is funded in part by SURA grant no. CNF19-04, NSF grants CCF-1439079, by NASA grant no. NNX15AU39A, ODU's Scholarships: Modeling & Simulation and Dominion Power and the Richard T. Cheng Endowment.

Outline of presentation

- Introduction and computer science context
- Nuclear physics context
- Goals of this project
- Project progress and accomplishments
- Future of the project
- Evolution of CNF
- Summary

Students

Current Work:

1. Christos is PhD student. — tessellation (including multi-scale graded)

2. Angelos is undergraduate student — software portability and ease-of-use: Docker, Jupyter, etc

Next Step: when it comes to multi-scale & graded meshes/grids can list

1. Joi Best (Mater level student)
2. Kevin Garner, PhD student (customize visualization plugins —coordinate with Nicolas Polys at VT)
3. Polykarpos Thomadakis, Machine Learning (along with Angelos).

Why Next Generation Imaging/Tessellations?

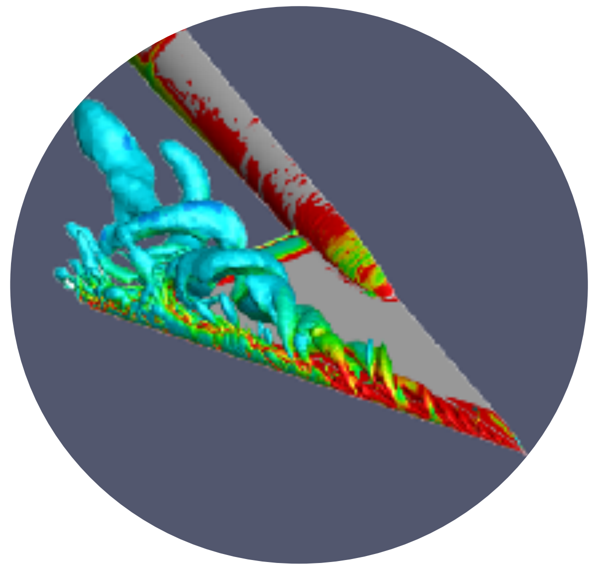
- "Large amounts of raw data (~1 PB per week) will need to be analyzed to provide the experimental input to 3D nucleon imaging".

– **Implicit representation using Imaging**

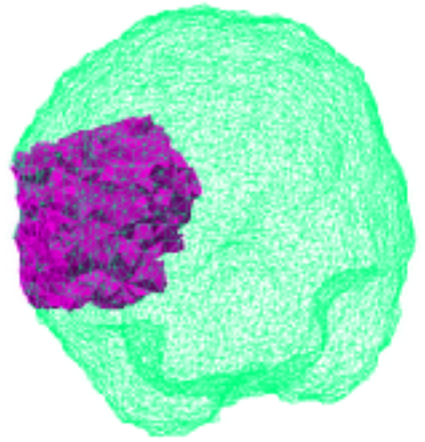
– "The production of experimentally determined distribution functions will involve substantial computation in order to derive the most probable distributions and to estimate their uncertainties."

- Image tessellation can help **focus computational resource** only where they are needed most!

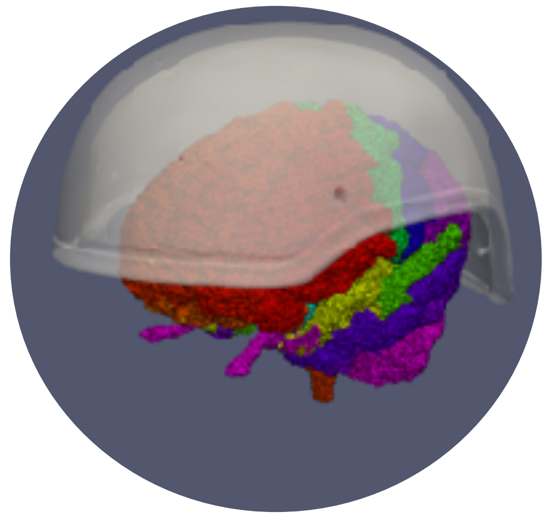
How? Leverage Imaging at CRTC @ ODU



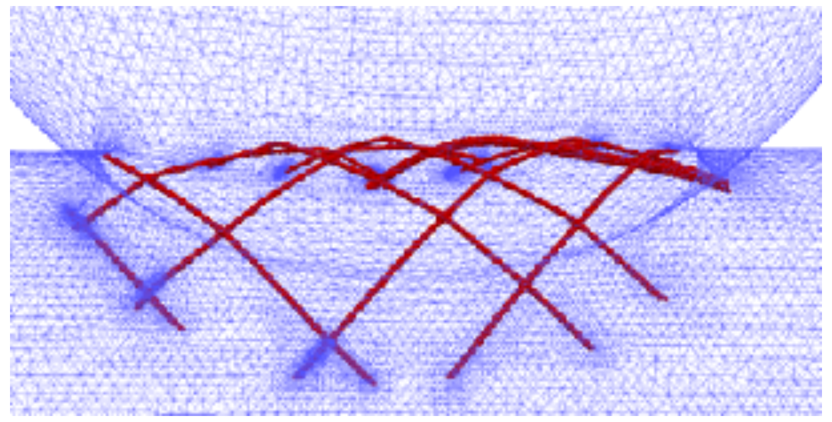
Extreme Scale FE mesh generation
- Conventional CMOS machines
- Quantum computing

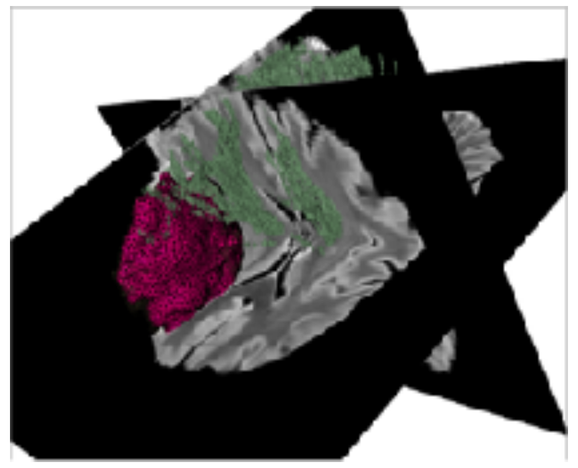


Real-Time I2M conversion
- 30 to 40M elms/sec. using about 1K cores



CAD- and Image-driven applications
- Traumatic Brain Injury
- Blood Flow Diversion in Aneurysms/Stents



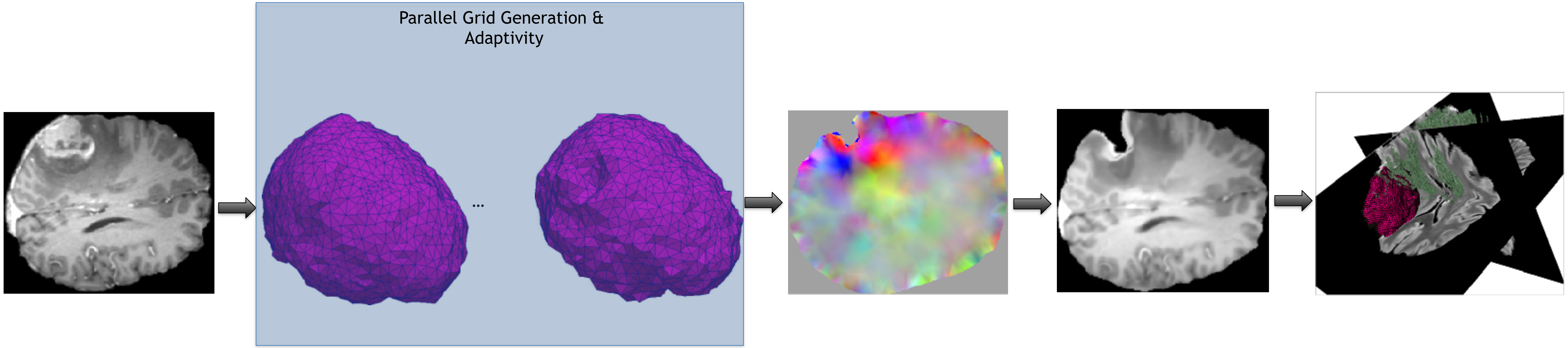


- Real-Time Deformable Registration

Perspectives on Scientific Computing for Medical Imaging (December, 2018)

Nikos Chrisochoides
Center for Real-Time Computing (CRTC)
Computer Science, ODU

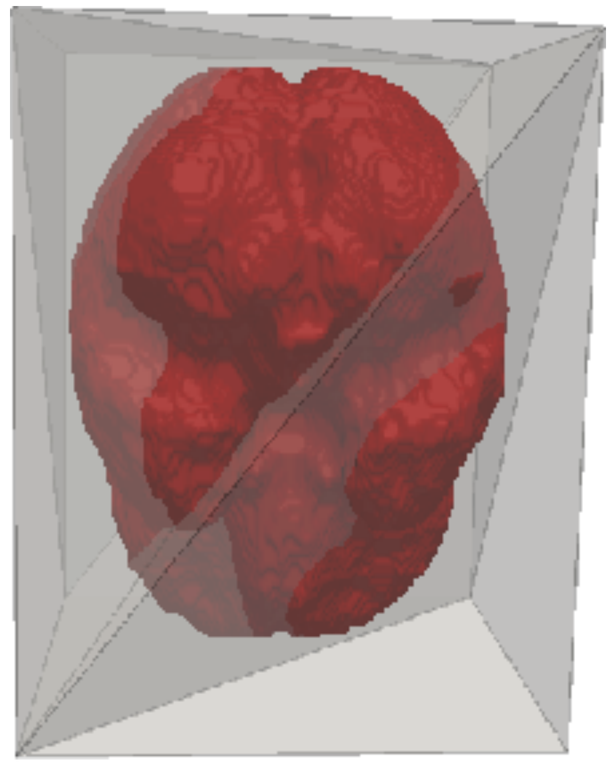
Wiki: https://cepm.cs.odu.edu/
Email: npchris@gmail.com

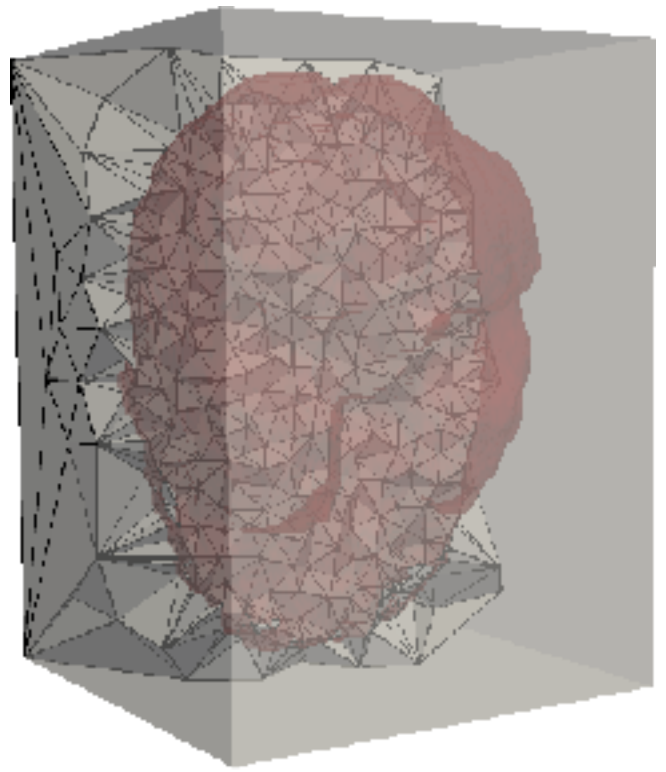


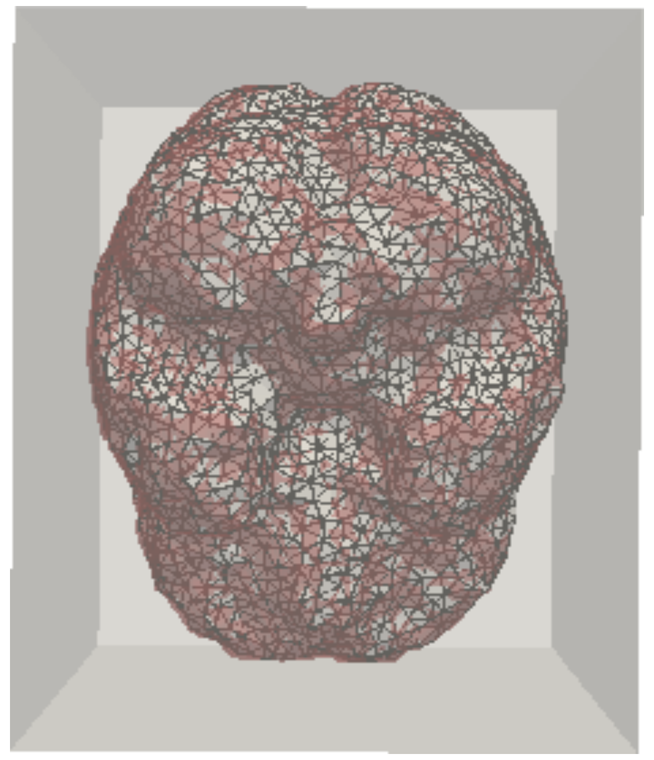
What? Use Parallel Optimistic Delaunay Meshing

Input: Segmented Image

Output: 3D (4D) discretization of the region of interest





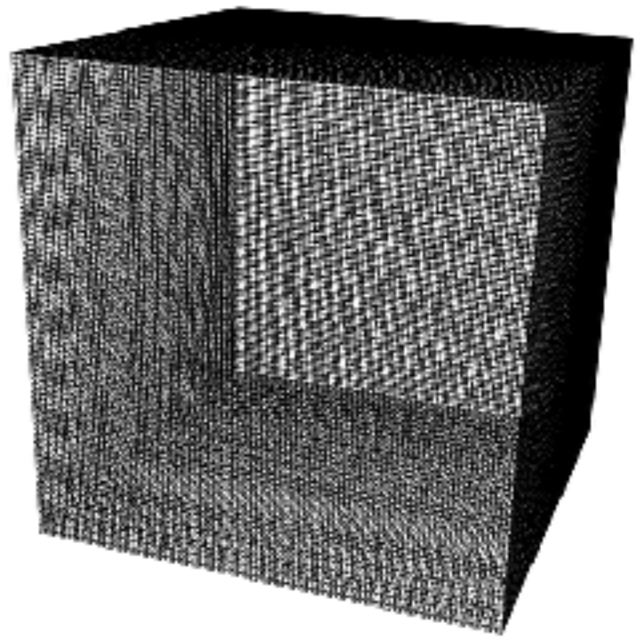


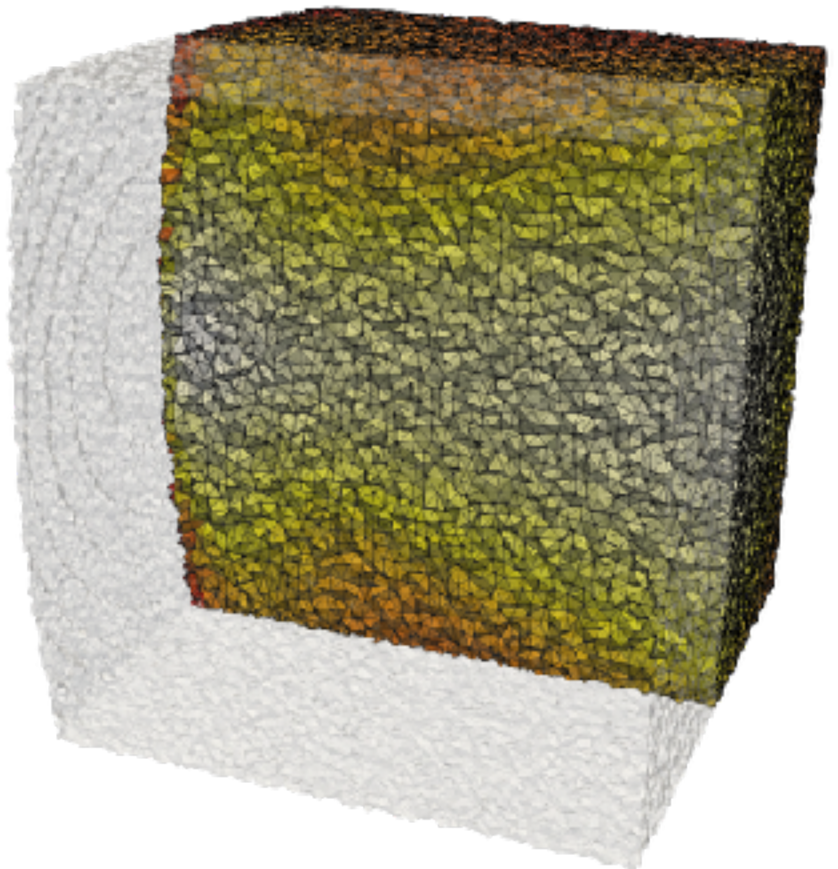
CNF (example) :

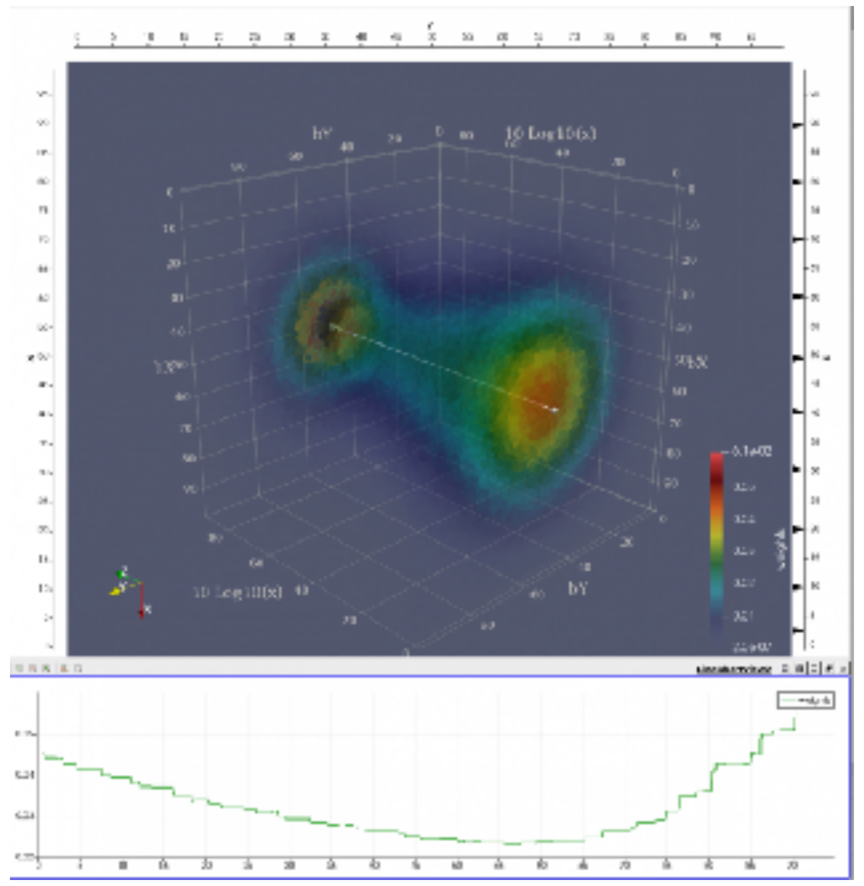
3D probability matrix

3D mesh

post-processing

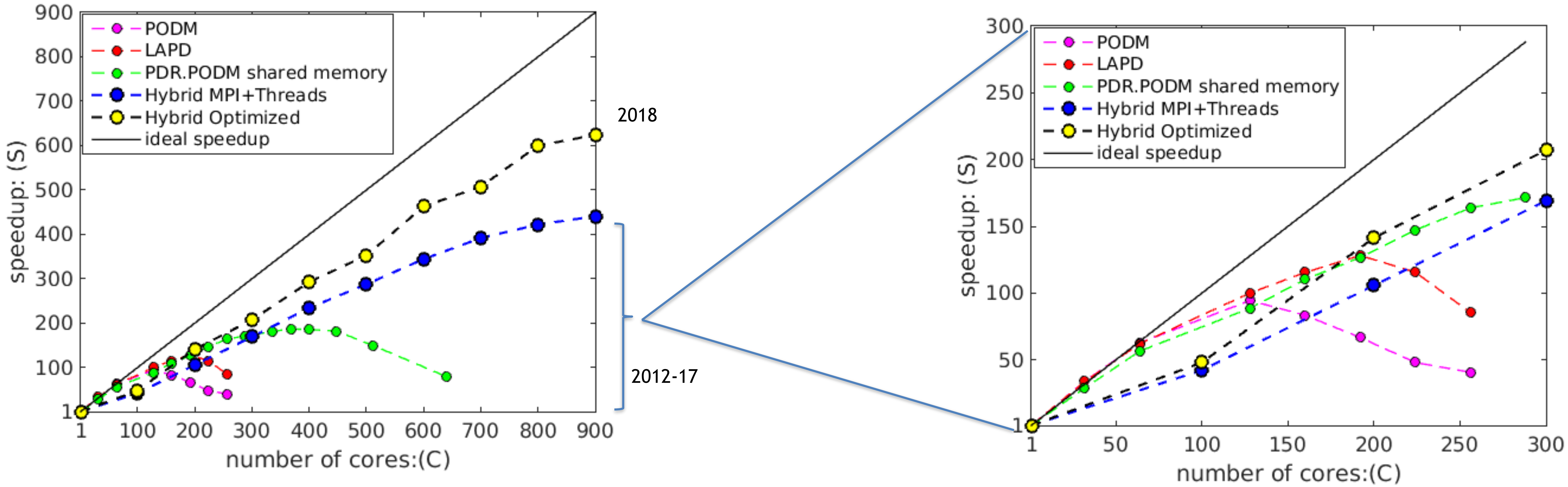




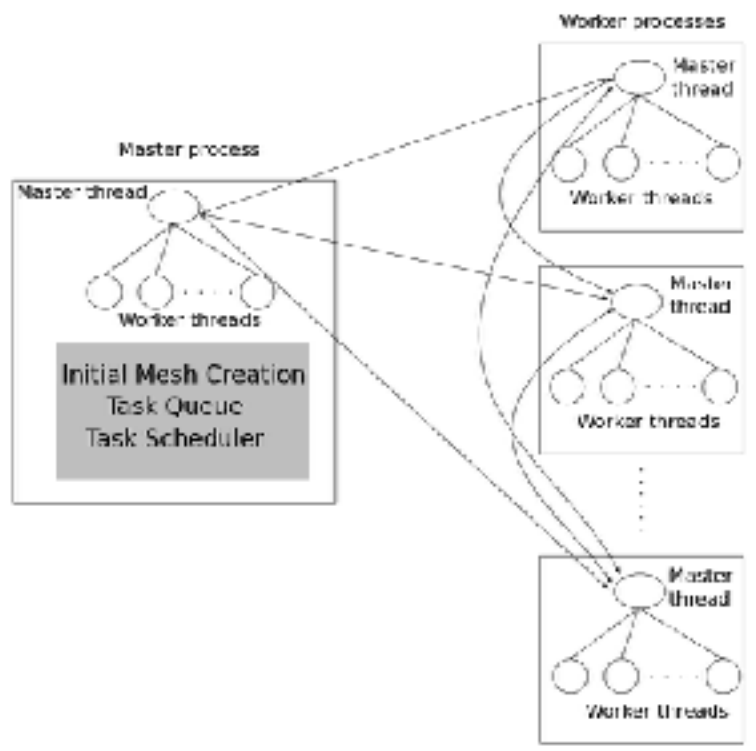


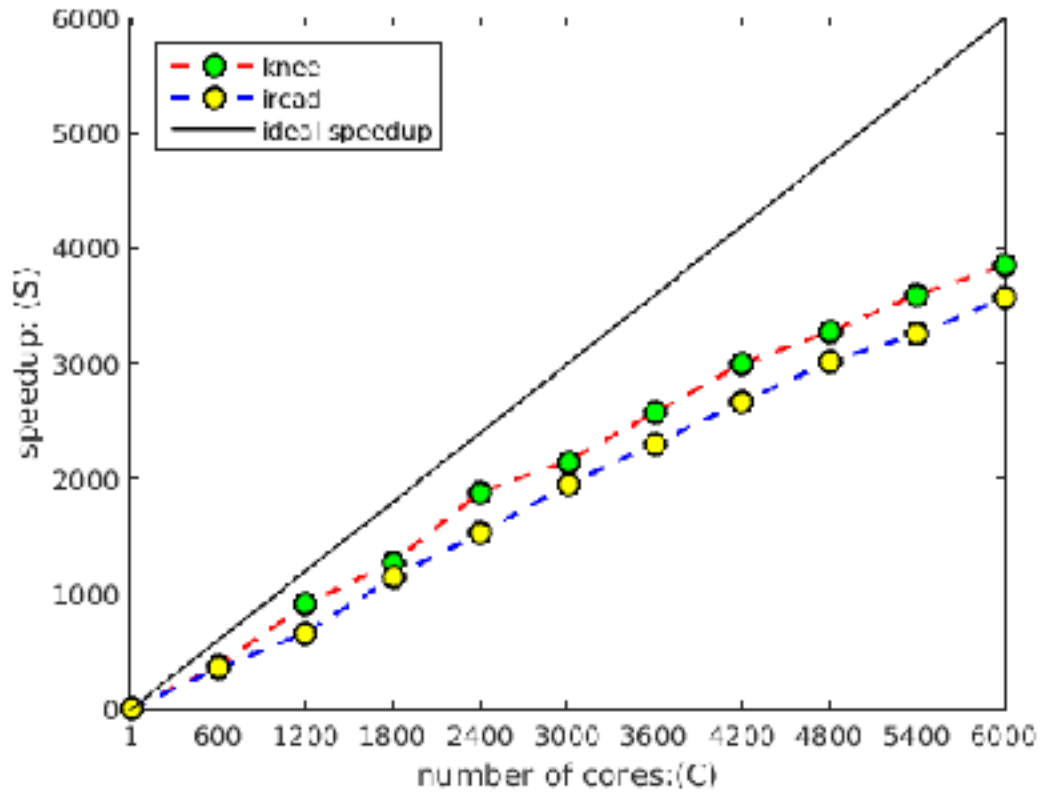
Gagik Gavalian (Jlab)

~70% parallel efficiency (w/o load balancing), for 300 to 900 cores



~66% parallel efficiency (**w/o load balancing**) for

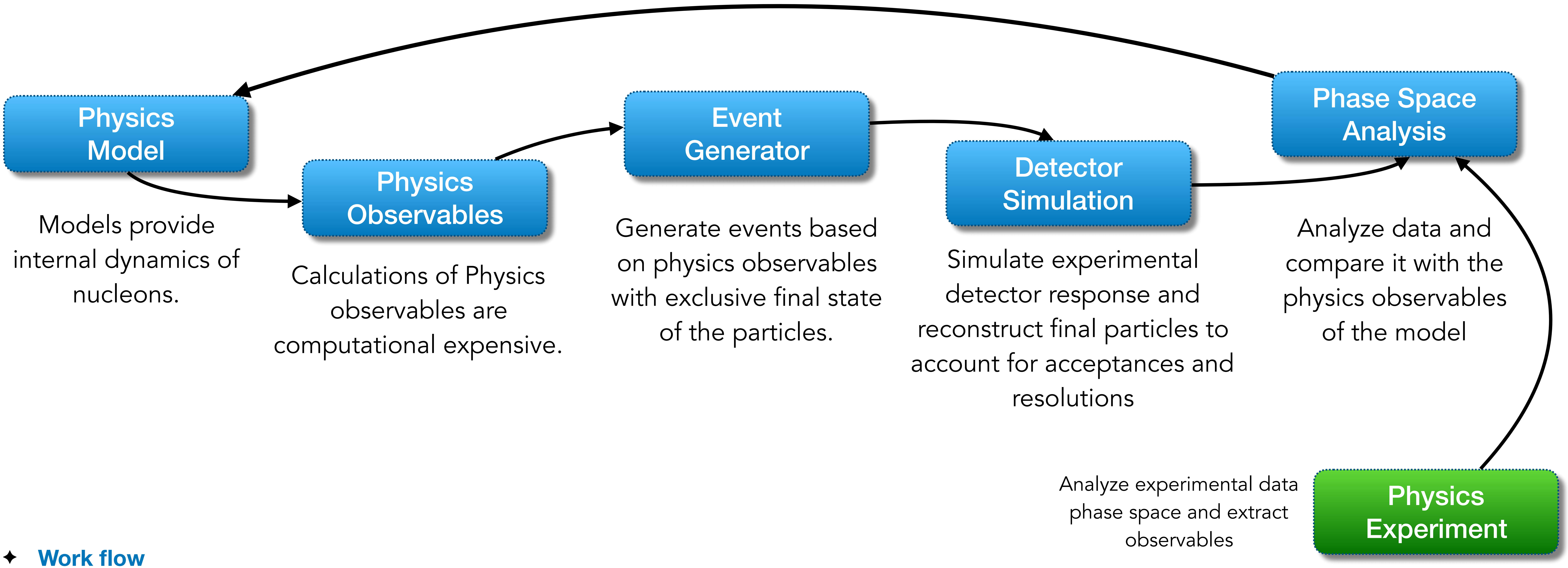




Nuclear physics: Software

- **Nuclear Physics**
  - Using same technology used 30 years ago
  - Haven't adopted new programming paradigms
- **The world outside NP:**
  - New programming languages evolved to make it easier to develop and share code.
  - Visualization software has evolved significantly in the past decade.
  - High Performance Computing provides tools for speeding up the discovery process.
  - Many specialized languages came forward that let you do things more efficiently.
  - Specialized software for sharing and processing data.
- **Where do we go:**
  - Have to try using new tools and software platforms
  - Innovate in visualization and data presentation.
  - Use new ways for distributing and using software.

Nuclear Physics Work Flow

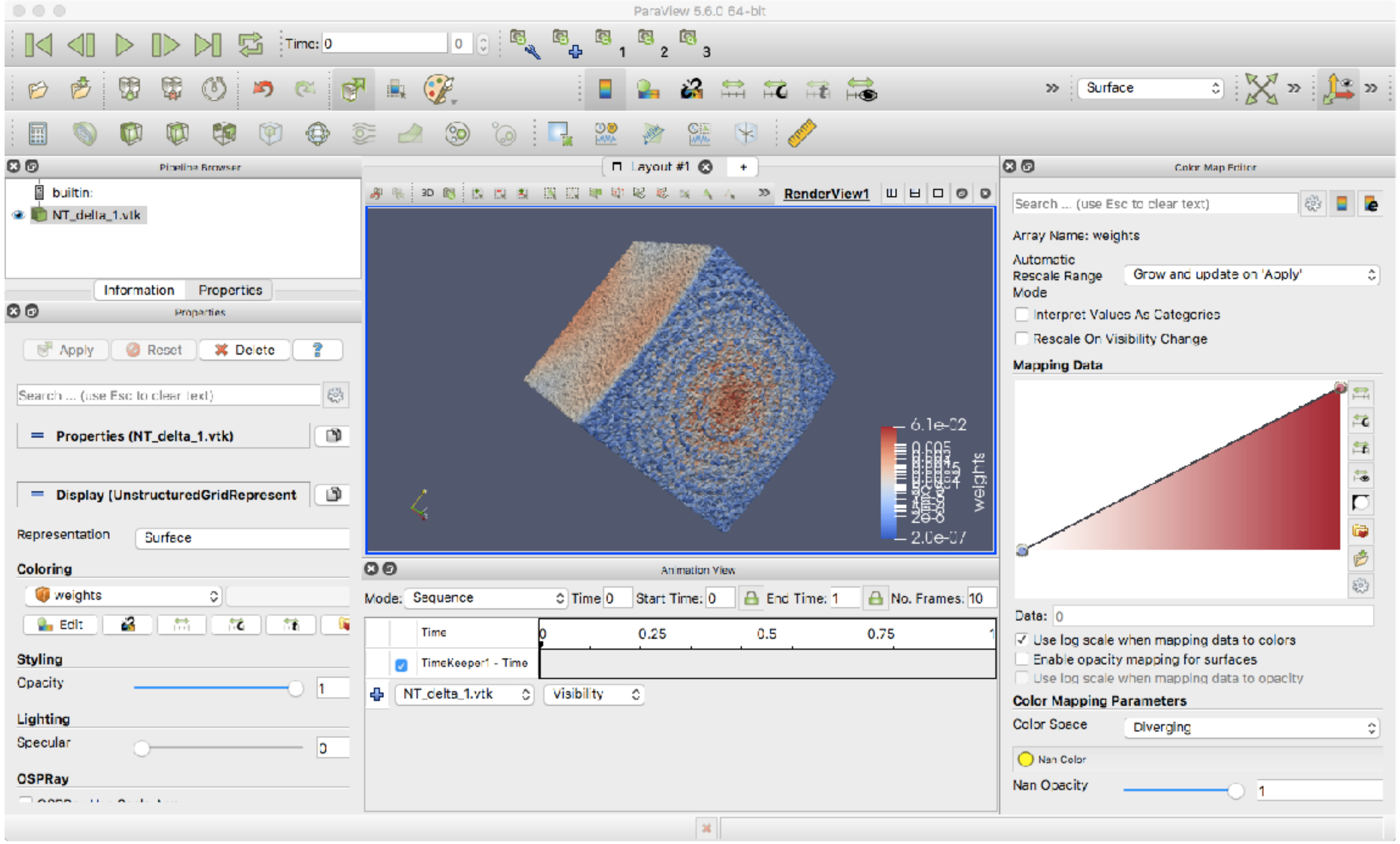


- **Work flow**
  - Every component of this workflow is developed by different groups (theorists develop models, experimental physicists develop event generators, analyzers develop their own comparison tools), no coherent framework exist.
  - Different visualization tools are used at every stage to validate calculations and compare experimental results with theoretical predictions.
  - No standard tools are available to substitute computationally intensive parts of the chain with parametrization and efficient iterative generation of models and observable.

- Visualization
- Simulation
- Data Analysis

Tessellation:

- Tessellation provides interface to open source visualization software.
- Visualization tools provide powerful tools for exploring the data:
  - slicing and projecting data
  - integration along lines and projections

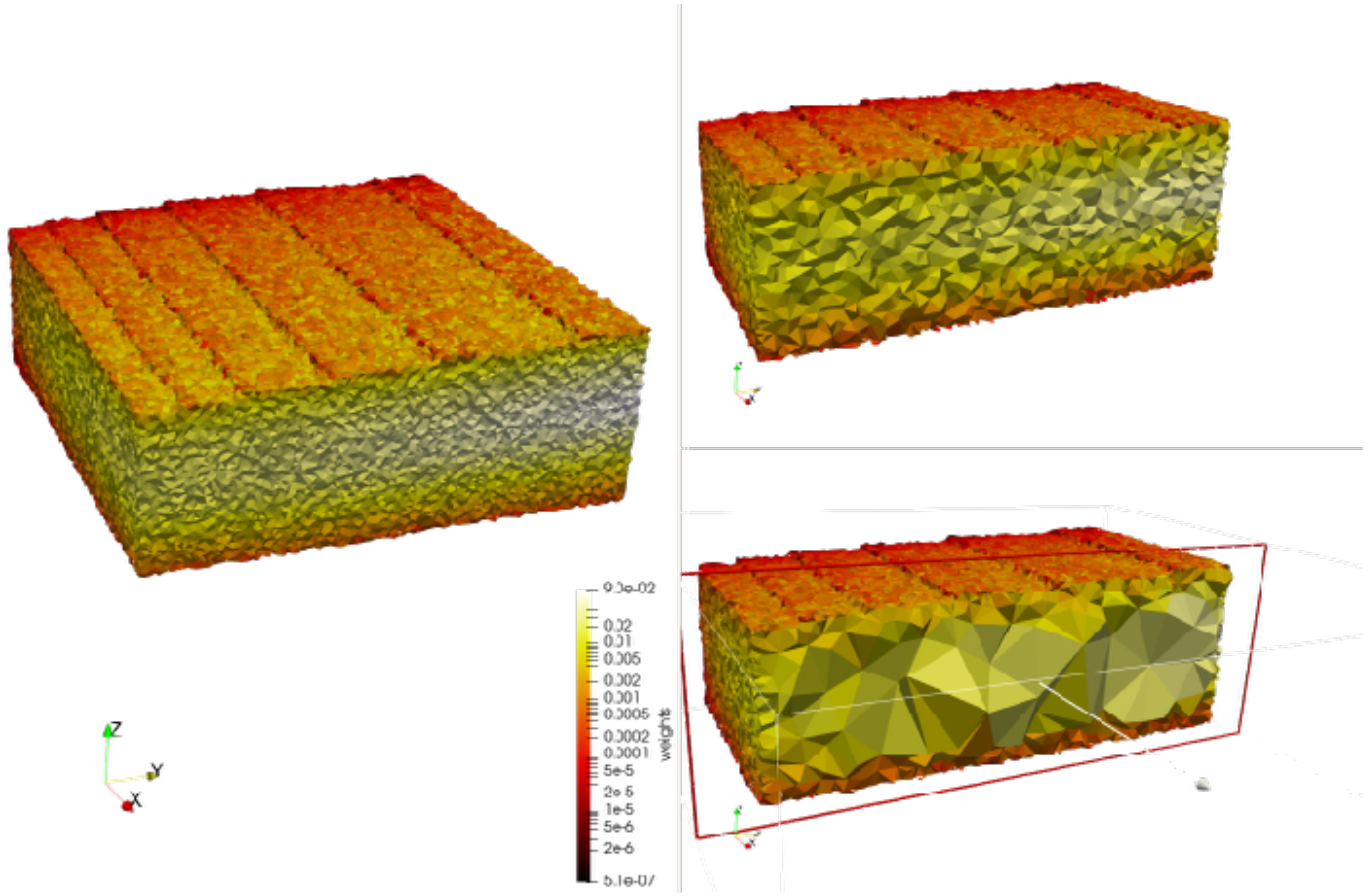


Simulation

Simulation:

- Tessellated object provide description of phase space in more compact form.
- Using tetrahedron to describe N-dimensional space is more memory efficient.
- Using tessellated description to generate random numbers for cross sections.
- Generating grids using PARTONS took 4 days (1M computations, for each point on the grid)
- Event generation (10M events) takes ~20 minutes
- Once the tessellated object is created for one model, can be used by everyone.
- The accuracy depends on fidelity of tessellation.

DVCS cross section as function of x,t,phi



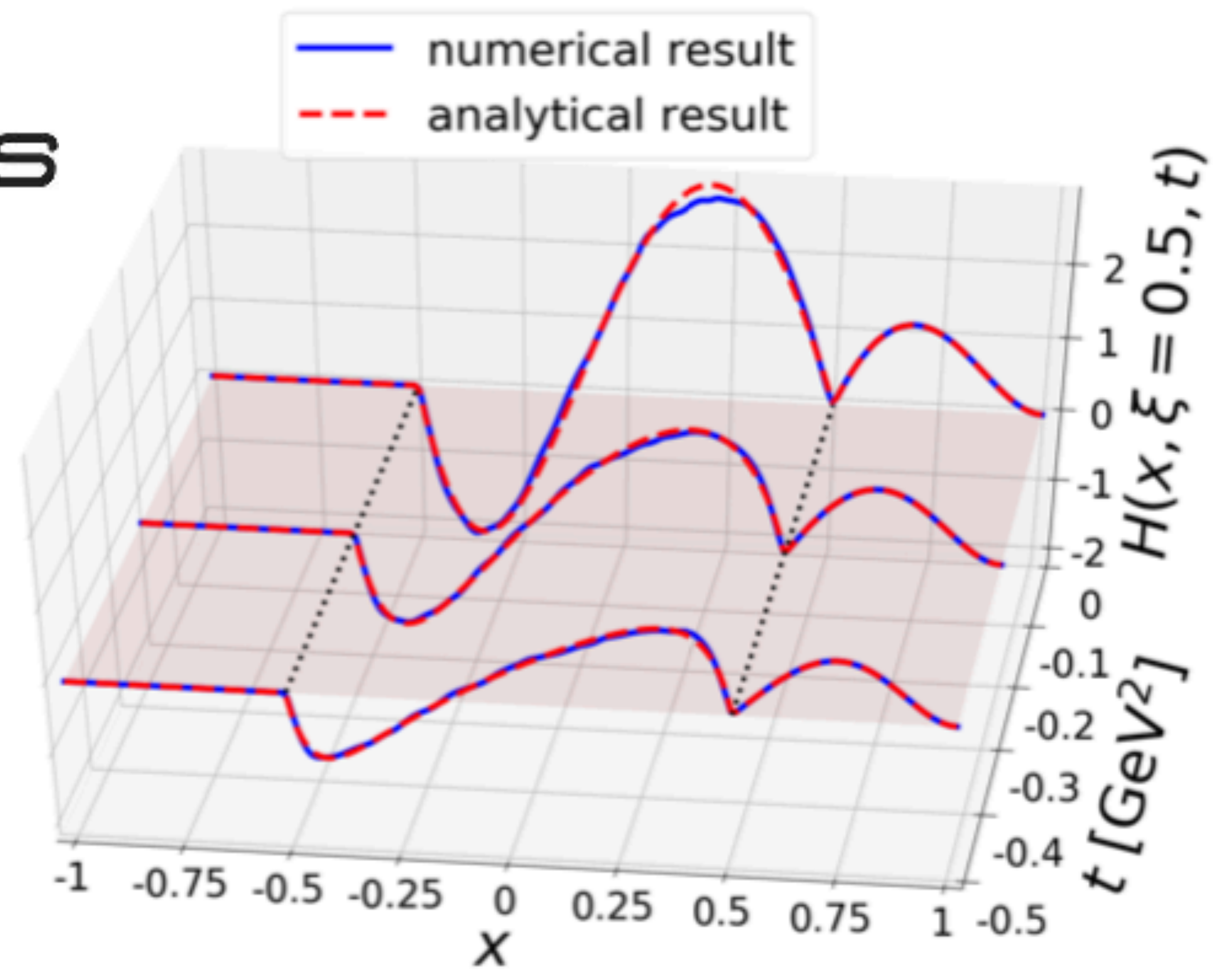
Data Analysis

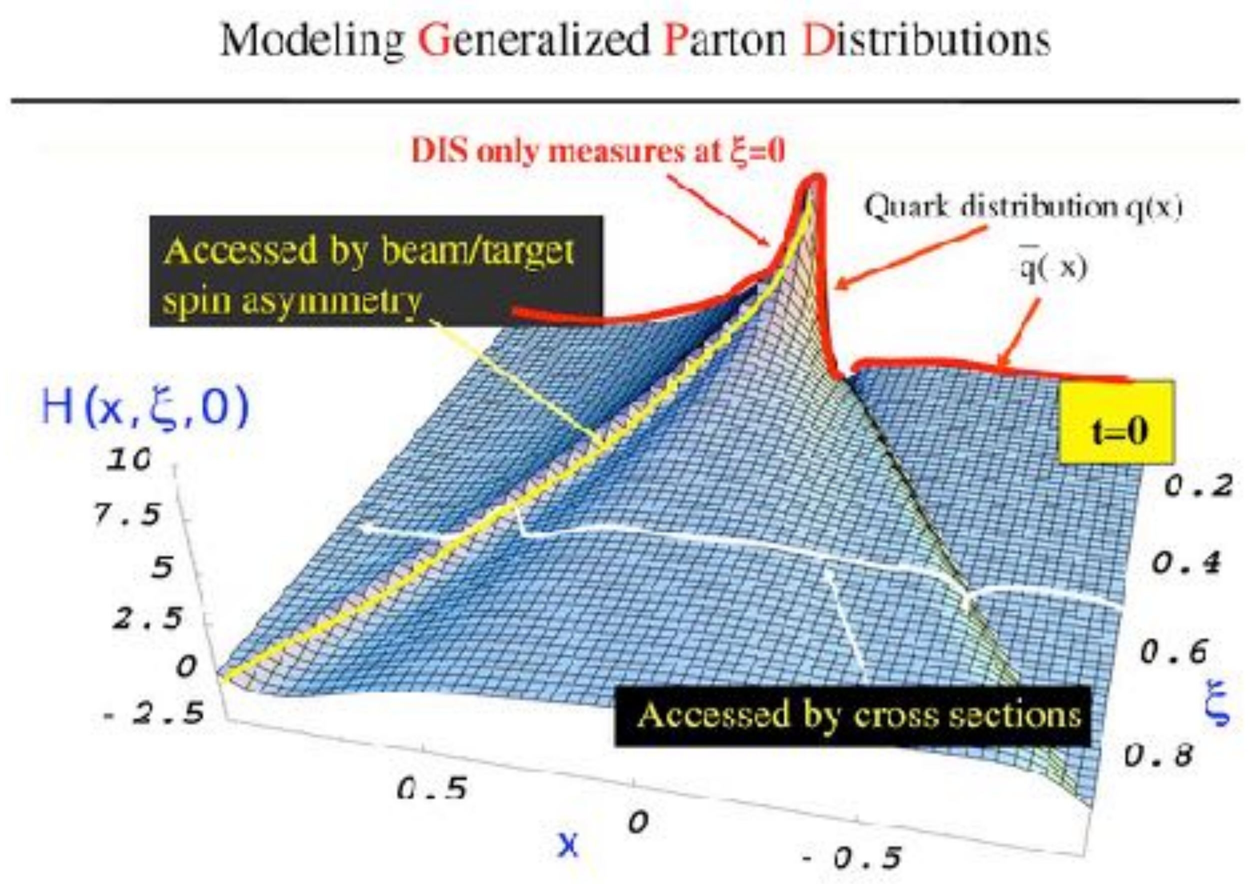
Data Analysis:

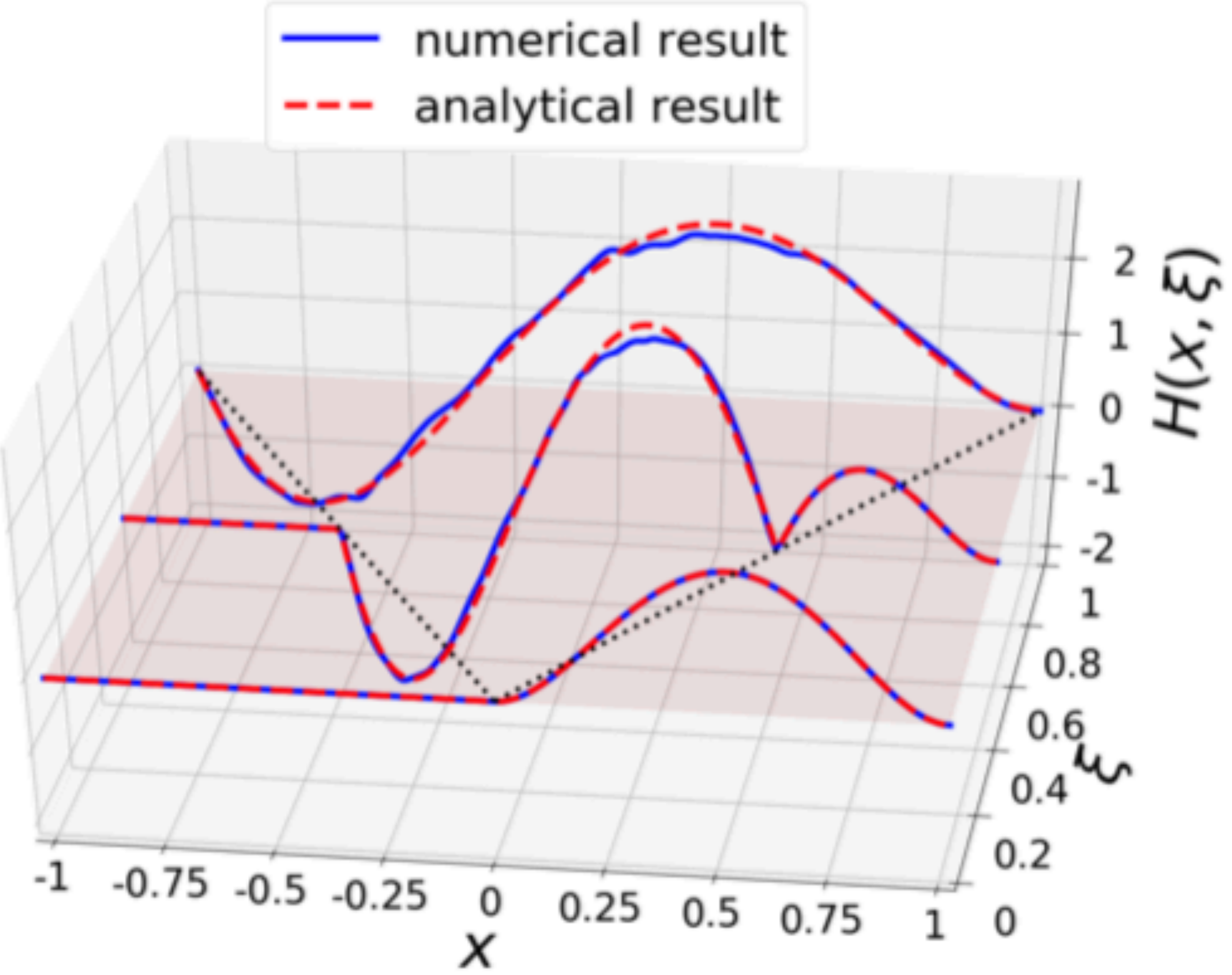
- ❑ Experimental results can be presented as tessellated object in N-dimensions
- ❑ Theoretical models can be used to simulate phase space of experiment
- ❑ Experimental observables can be compared with theoretical predictions in N-dimensions.
- ❑ Using visualization tools to explore difference between the models and experimental data.

tools (PARTONS)

PARTONS is a C++ software framework dedicated to the phenomenology of Generalized Parton Distributions (GPDs). GPDs provide a comprehensive description of the partonic structure of the nucleon and contain a wealth of new information. In particular, GPDs provide a description of the nucleon as an extended object, referred to as 3-dimensional nucleon tomography, and give an access to the orbital angular momentum of quarks.



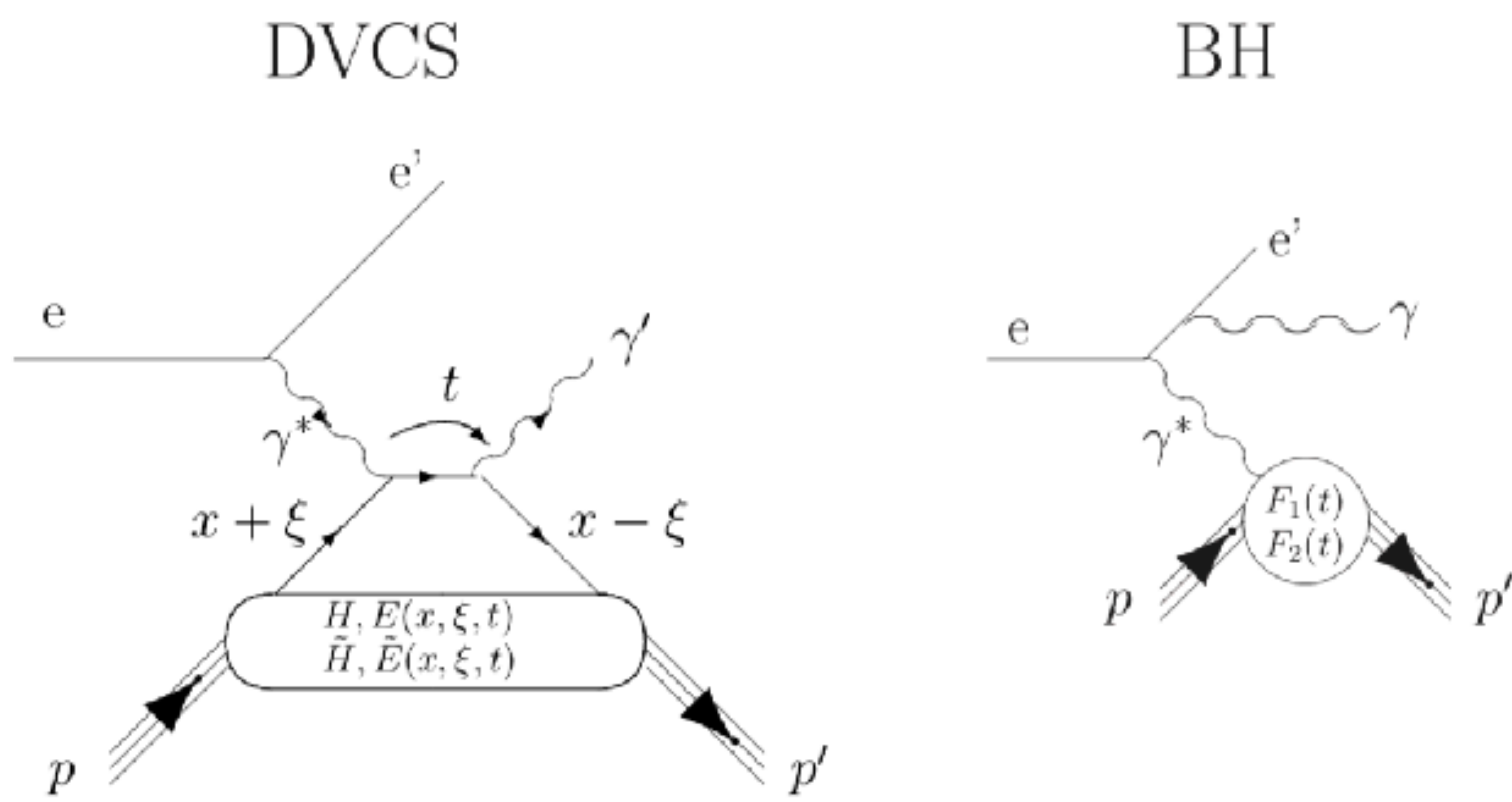


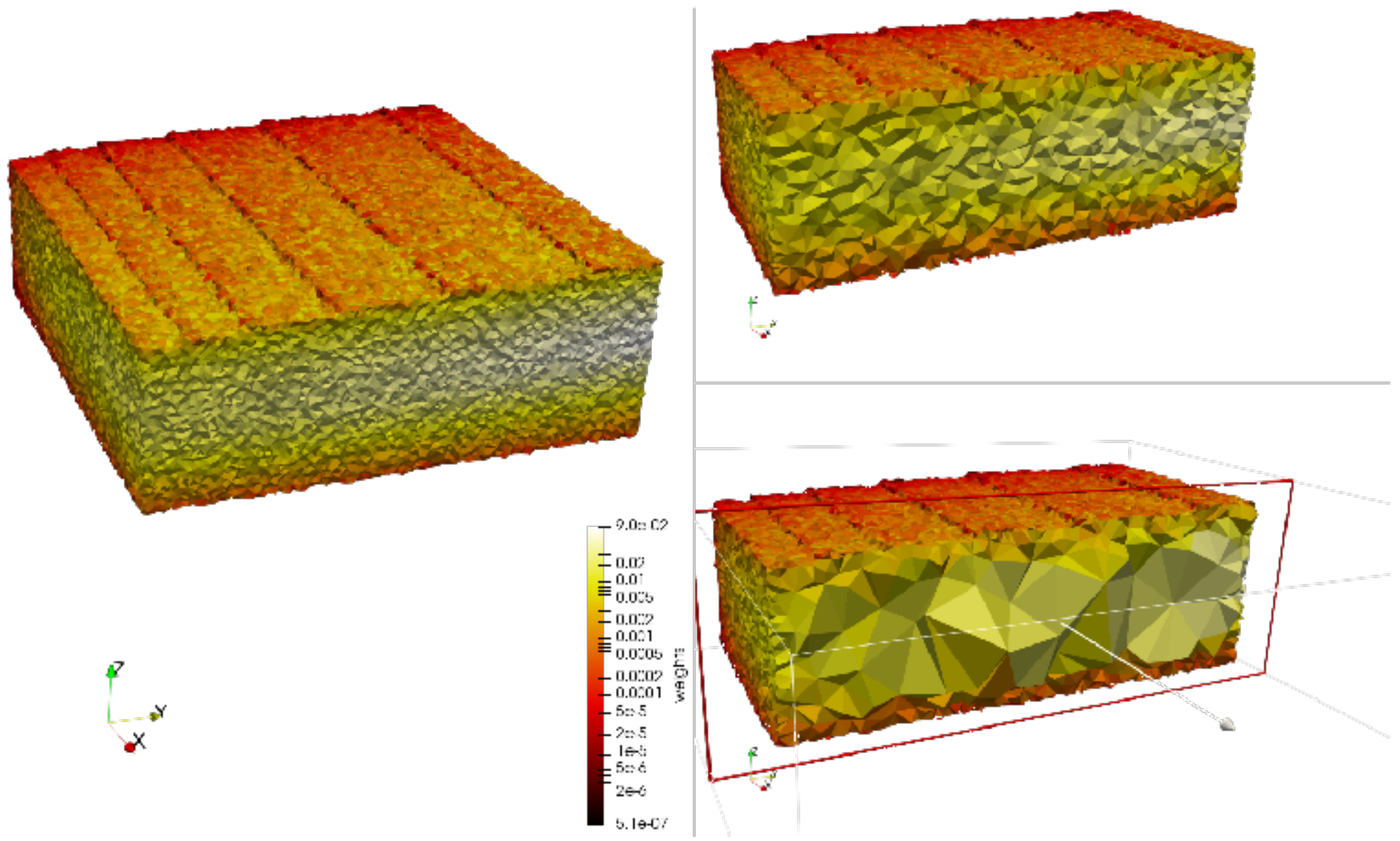


- **PARTONS**
  - Generates quark distributions for given parameter space.
  - Generates Generalized Parton Distributions (includes many models)
  - Generates physics observables for given grid (such as cross sections and asymmetries)

Tessellation

- PARTONS software was used to generate Deeply Virtual Compton Scattering cross sections as function of Q2, x, and phi.
- This process probes the internal structure of the proton, to learn about quark orbital momentum inside the protons.
- Generated GRID was processed with tessellation software to produce 3-D mesh for ParaView.
- **Tessellated Mesh in ParaView:**
  - sliced view of distribution with intensity color map
  - plot distribution along any line in space.
  - plot integrals for any slice and projection of density distribution.
- **Using meshes for simulation:**
  - tessellated objects can be used to generate random numbers following density distribution.
  - the process is very fast compared to calculating convoluted integrals numerically (in case of DVCS cross sections)
  - tessellated physics models can be shared with experimental physicist for easy particle simulations.

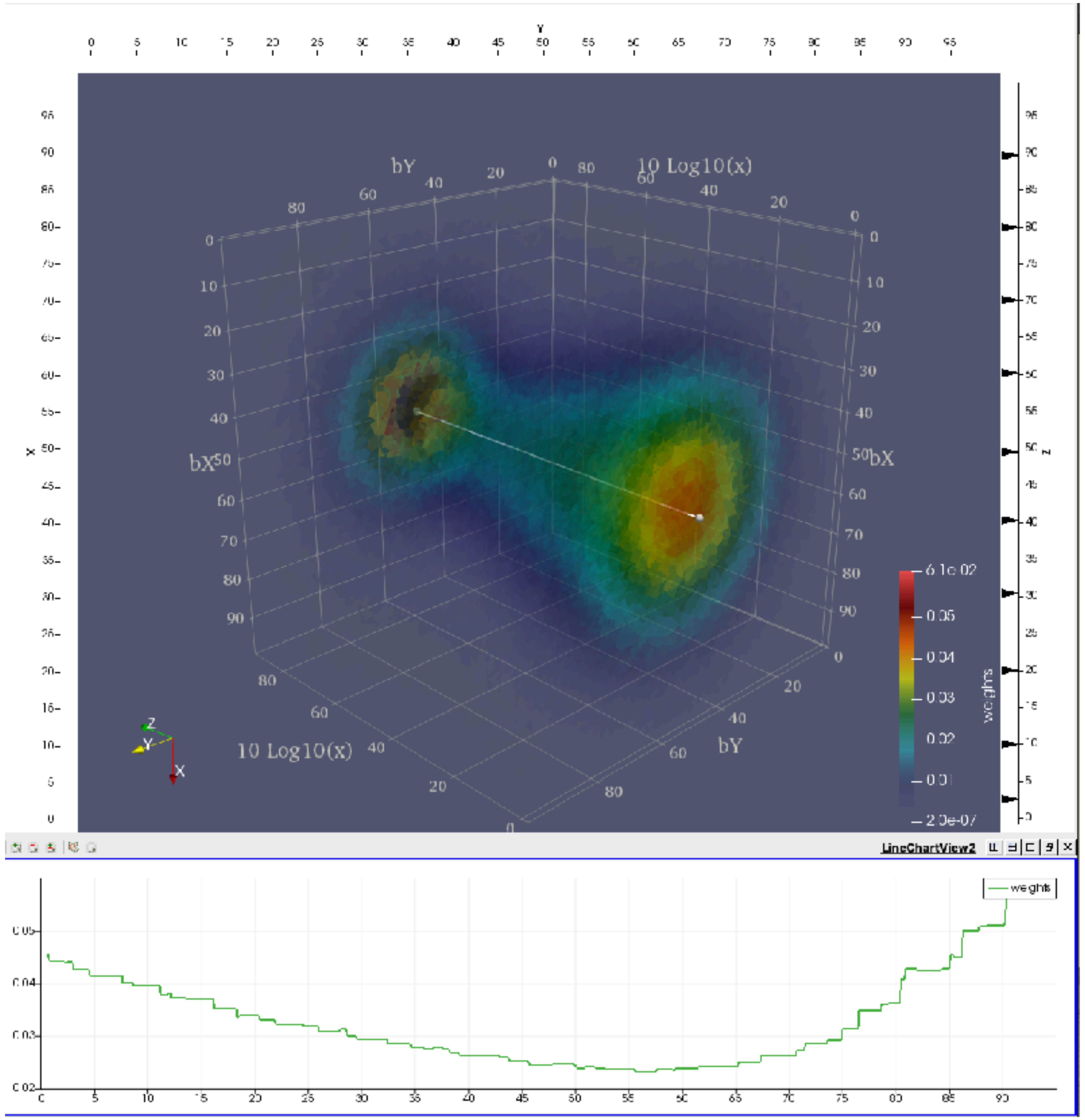




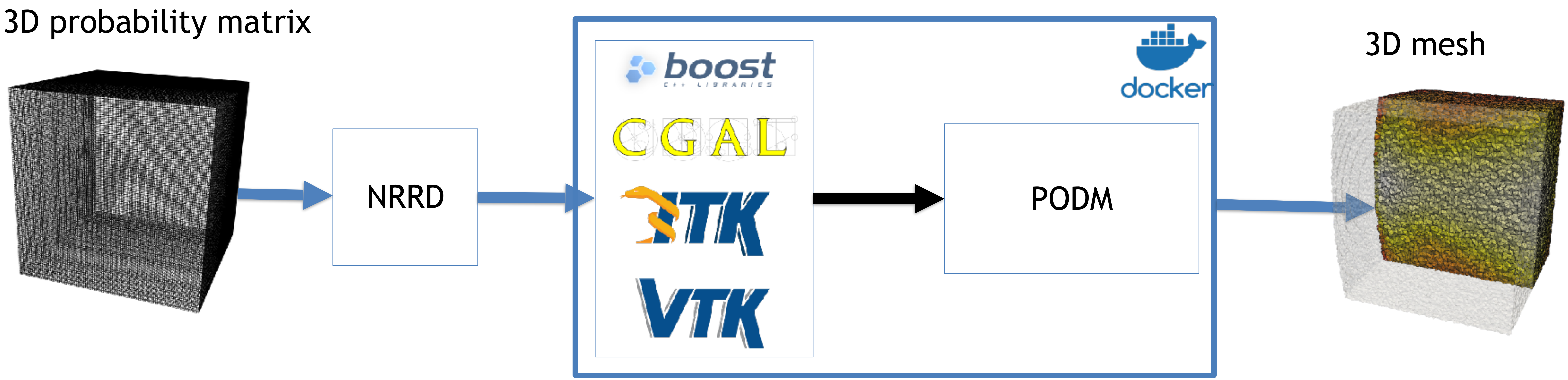
Gagik Gavalian (Jlab)

Tessellation

- PARTONS software was used to generate u-quark density distribution as a function of impact parameter.
- Generated GRID was processed with tessellation software to produce 3-D mesh for ParaView.
- **Tessellated Mesh in ParaView:**
  - sliced view of distribution with intensity color map
  - plot distribution along any line in space.
  - plot integrals for any slice and projection of density distribution.
- **Using meshes for simulation:**
  - tessellated objects can be used to generate random numbers following density distribution.
  - the process is very fast compared to calculating convoluted integrals numerically (in case of DVCS cross sections)
  - tessellated physics models can be shared with experimental physicist for easy particle simulations.

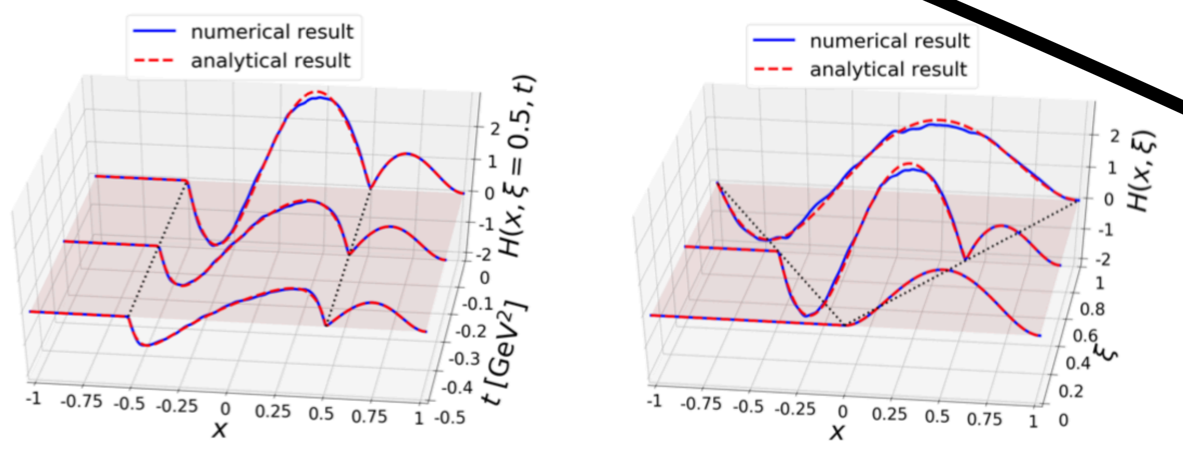


Parallel Optimistic Delaunay Mesh Generation



FULL Chain

PARTONS



PARTONS Generate:

- quark distribution functions
- GPD's (H,E,Ht,Et)
- Beam Spin Asymmetries
- Cross Sections (BH, DVCS, INT)

ANY USER PROGRAM

OTHER CNF Proposals

Future:

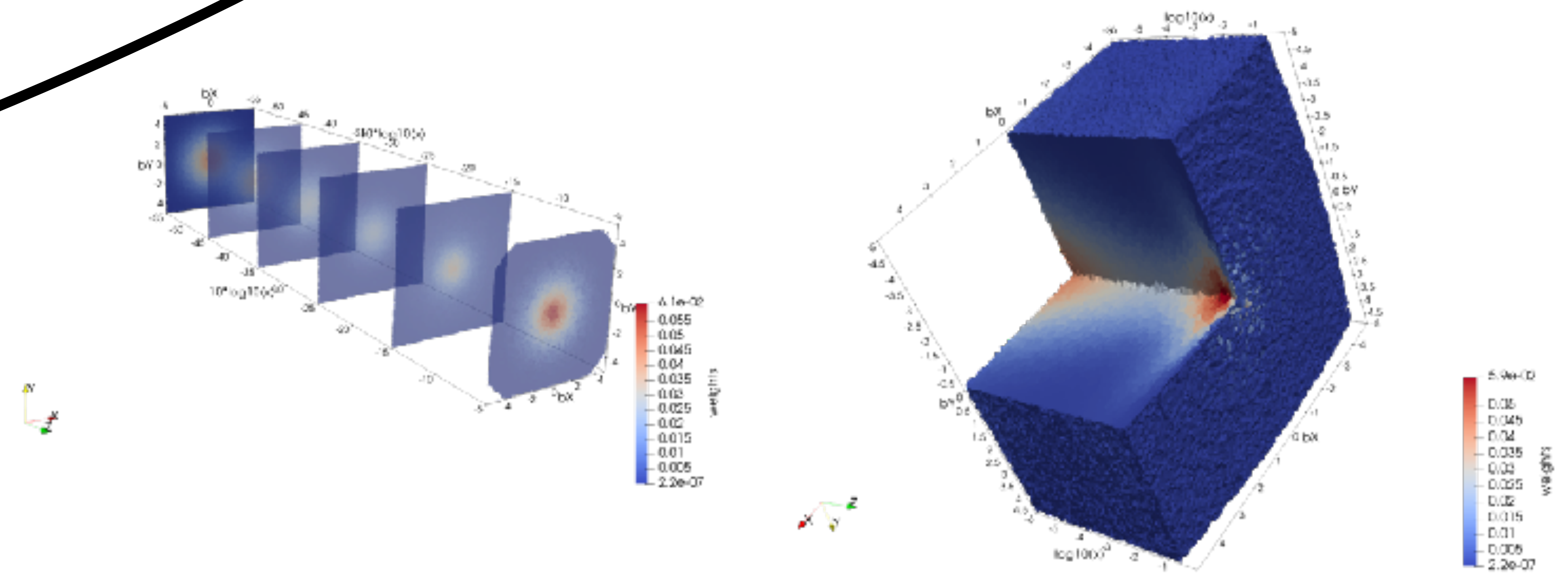
- user programs can use this chain
- other proposals can take advantage the software.

CNF_I2M:

- convert GRID to NRDD/DICOM
- generate tessellated file (VTK)
- software is available through docker

CNF_I2M
Tessellation
ODU
Docker

ParaView



ParaView:

- plot slices of tessellated image
- boolean operations with planes and objects
- calculate integrals over lines or planes
- custom Python views with fully programmable data analysis routines.
- provides most customizable data visualization plugins (user programmable).

Future of this project

Tessellation:

- ❏ Extend software to do tessellation in N-dimensions. We can store cross section information for more complex reactions.
- ❏ Improve tessellation fidelity with using density as step function.
- ❏ Implement tools for Monte-Carlo generation based on tessellated objects.

Visualization:

- ❏ Provide custom data analysis views in ParaView using python plugin system.
- ❏ Implement several analysis plugins for experimental and theoretical data.

Work Flow:

- ❏ Package tessellation software and PARTONs in one docker container for ease of use.
- ❏ Include JUPYTER in docker, provide examples how to run theoretical calculations and tessellation software.
- ❏ Implement tessellated object visualization using VTK.js package.

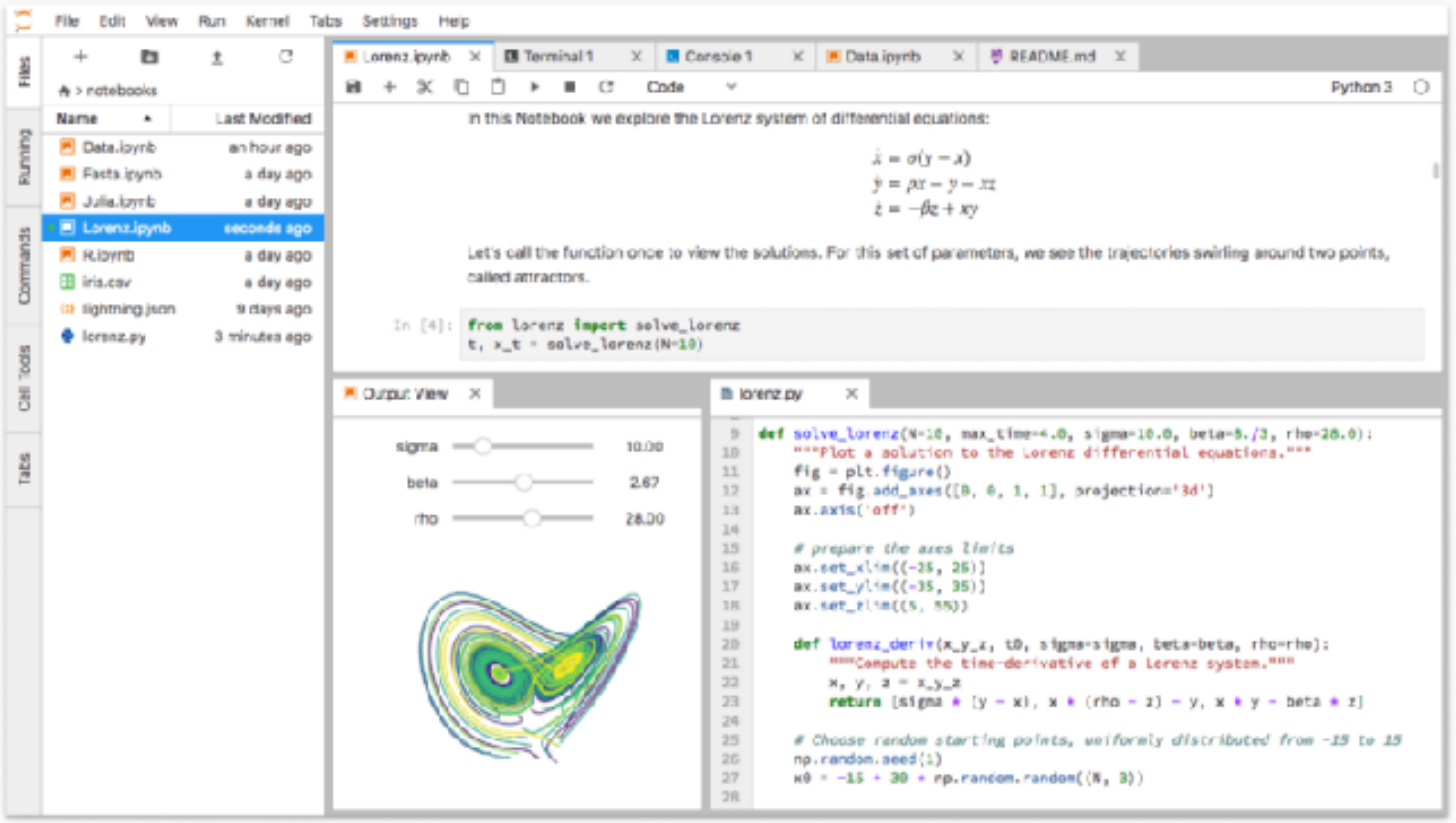
Future Developments&Collaborations

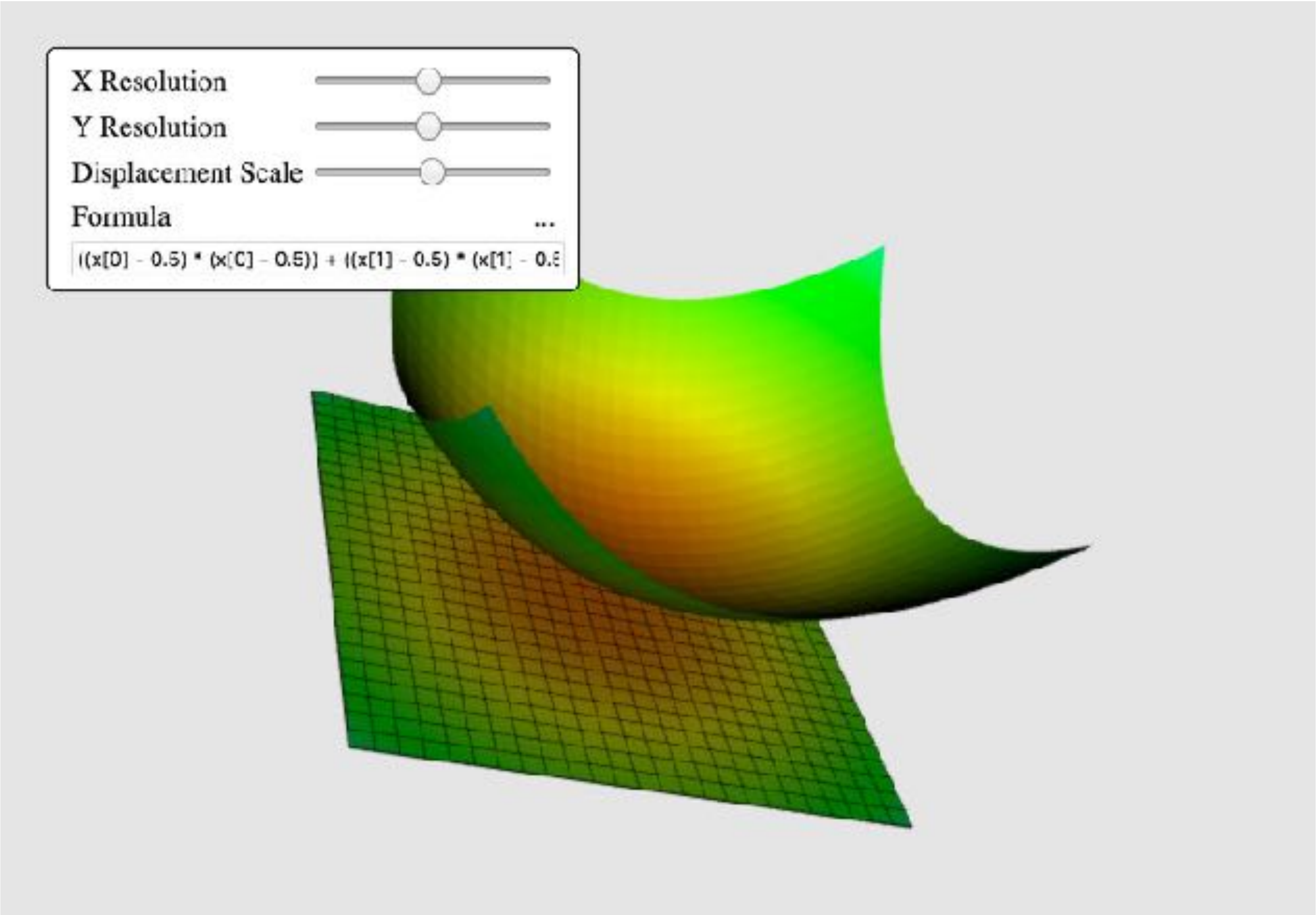
✦ New Approaches:

- software components have to be tied together to work within same environment using same technologies.
- these new encapsulated environments allow sharing codes and data, and providing consistent familiar workflow.
- Jupyter allows integration of different tools into coherent programming environment, where computation and visualization can co-exist.
- Docker usage make easy (no compilation, no installation) to distribute libraries and frameworks.

✦ Going Forward (with this proposal):

- it will benefit the project to bring all proposals under same umbrella.
- share tools and environments for developing and distributing code.
- new ideas can be shared and discussed.
- everyone will benefit.





Summary

- Used PARTONS Software package to generate quark distributions and physics observables.
- Developed a software for tessellating density distribution functions and presenting them in ParaView. (http://www.cs.odu.edu/crtc/cnf_project/index.html)
- Packaged software in docker containers and are runnable on any system (no installation or compilation required)
- Future Plans:
  - Provide web interface to run PARTONS (or any other software) to produce physics observables using Jupiter notebooks.
  - Develop tools for tessellated distribution visualization using vtk javascript library.
  - Look into collaborating with other projects that can leverage our already developed software infrastructure.

BACKUP SLIDES

Goal of the proposal

- **Goals:**
  - Provide tools for physicists to visualize theoretical data and make comparisons of different models.
  - Provide software infrastructure to generate events for experimental setups to test and validate experimental results.
  - Develop software for comparing experimentally measure observables with theoretical models using tessellation of phase space.
- **Plan:**
  - Process output of theoretical model calculations (PARTONs GPD model) for generation of NRDD/DICOM images and produce segmentation.
  - Generate N-dimensional sequence of tessellation, to be used for visualization (using industry standard tools, such as ParaView) and numerical integration.
  - Use tessellated objects to substitute computationally intensive parts of model calculations with much faster Monte-Carlo for phase space generation.
  - Provide conversion tool using Docker technologies for ease-of-use and portability.
  - Experiment with existing tools (Slicer-3D and ParaView) to visualize slices and projections of tessellated objects.