Verification of the Time Evolution of Cosmological Simulations via Hypothesis-Driven Comparative and Quantitative Visualization

Chung-Hsing Hsu, James P. Ahrens, Jonathan Woodring and Katrin Heitmann

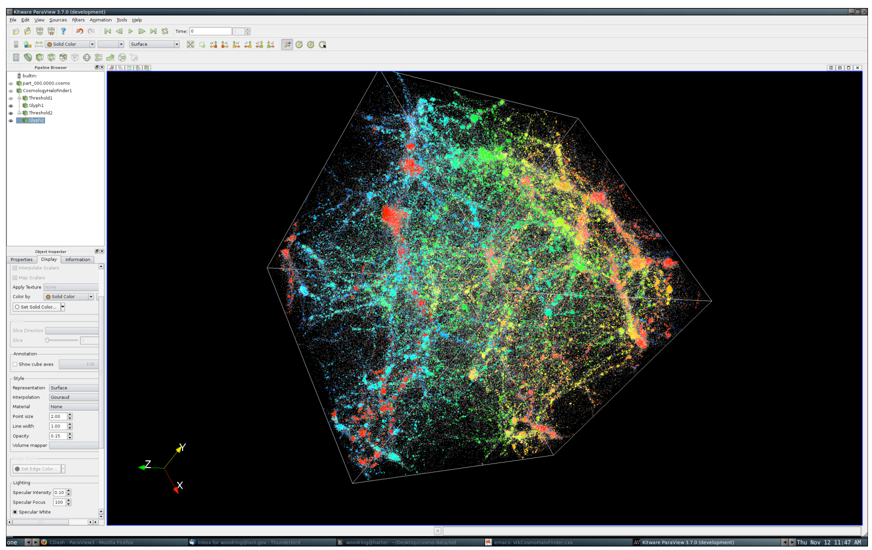
Los Alamos National Laboratory

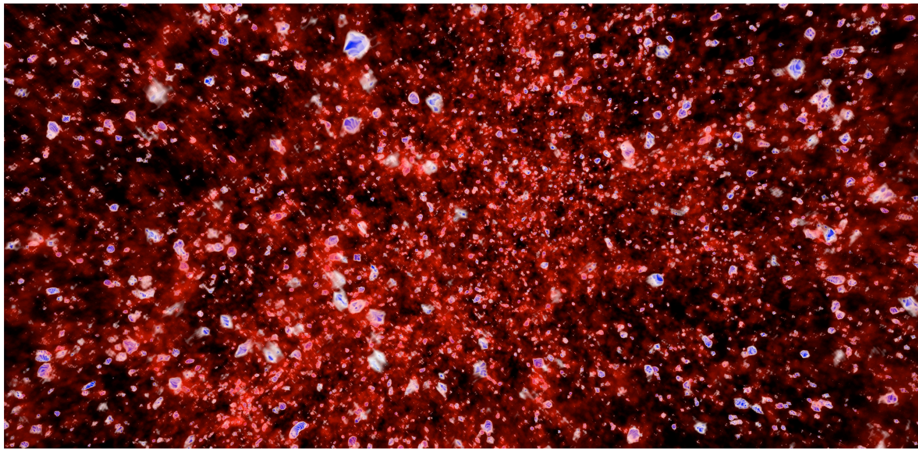
Executive Summary

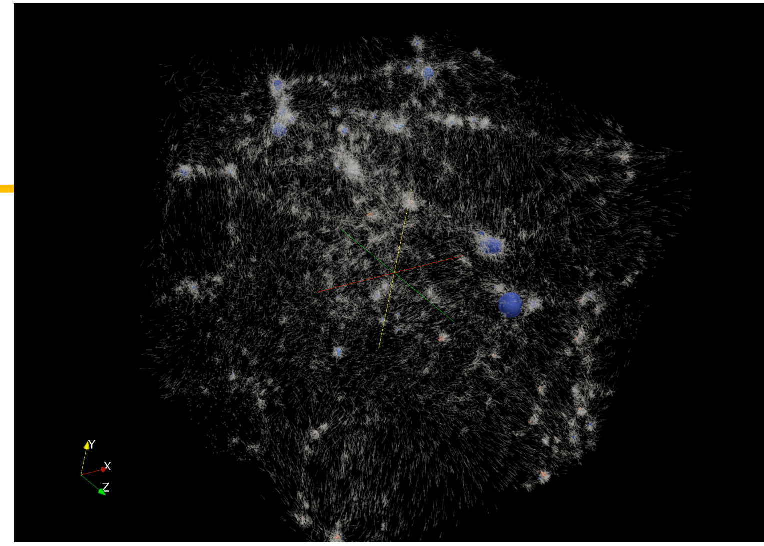
- **A structured interactive visualization workflow applied to a particular task by scientists that generated a scientific result**
  - The task: Code verification for cosmological simulations
  - The solution: An iterative comparative visualization workflow
  - The case study: The interactive application of the workflow to the task, and the scientific discovery that resulted from it
- **This is a documentation of this visualization workflow as a scientific process, rather than an art**
  - Ideally, this should be one of many workflows in a visualization workflow "cookbook"
  - When a given a particular task, a user or scientist can match the workflow that best fits to solve their problem

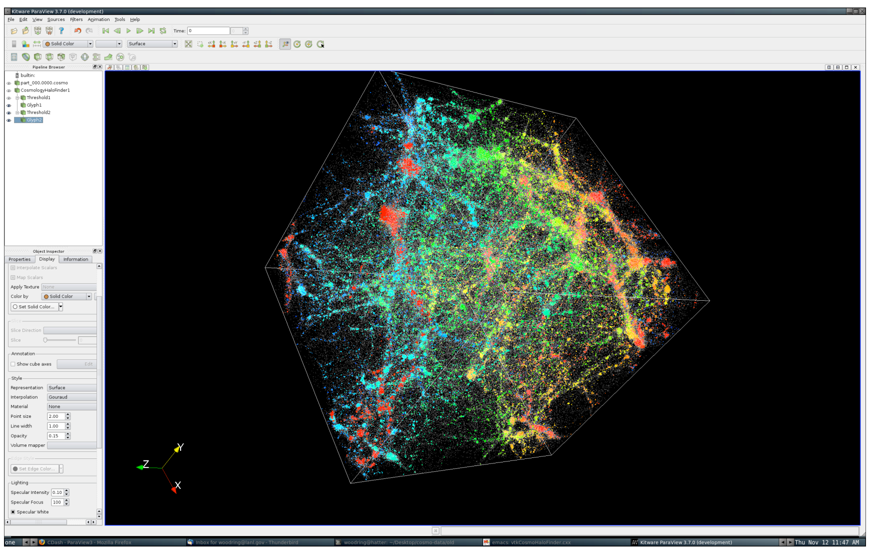
Cosmological Physics and Simulations

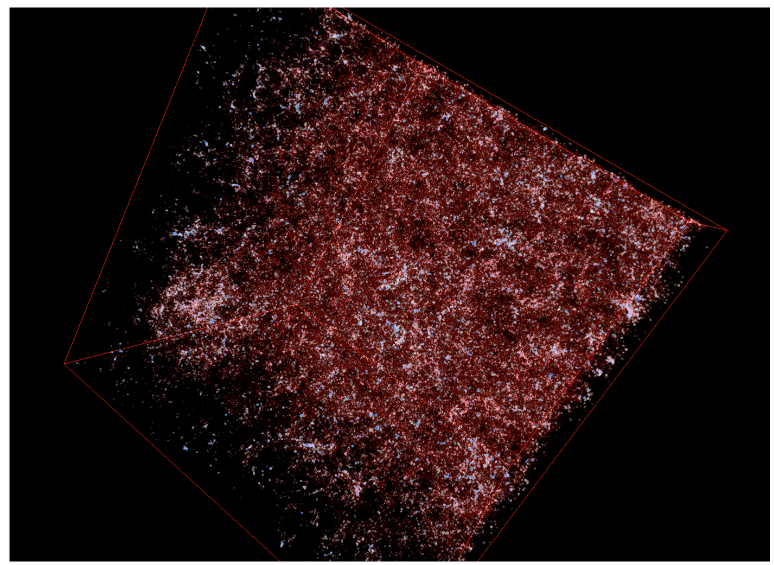
- **In cosmological theory, the universe is dominated by dark matter and dark energy – there is a lot of “unseen” matter out there that has gravitational effects on the “seen” matter in the universe**
- **Understanding the physics of dark matter and dark energy requires accurate predictions from simulation codes to interpret observational data**











Task: Cosmological Code Verification

- **GADGET-2, MC^2, and Enzo**
  - Each of these codes were independently developed by different institutions around the world
- **All three codes solve the same N-body problem: evolution of the dark matter distribution in the expanding universe**
  - Their underlying algorithms are different
- **Code verification in this context means:**
  - The algorithms are used to solve the model equations; running the simulations should produce the same results given the same initial starting conditions
  - If not, the cosmologist should understand why not and the limitations of the simulation
- **It is not trivial to verify that the codes produce the same results**
  - Cosmological simulations are highly non-linear, and the few numerically solvable analytic problems only provide hints to the accuracy and similarity of codes

Solution: Verification of the Codes by a Structured Comparative Visualization Process

- Register the codes

1. Define and refine features
2. Formulate/refine hypothesis about measurable differences between the codes
3. Test by Qualitative comparative visualization
4. Test by Quantitative comparative visualization

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Register the codes

- **Register the codes**
  - Codes are registered such that time steps and spatial coordinates are in agreement

1. Define and refine features
2. Formulate/refine hypothesis about measurable differences between the codes
3. Test by Qualitative comparative visualization
4. Test by Quantitative comparative visualization

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Define and refine features

- Register the codes

1. **Define and refine features**
   - A measurable feature is defined and extracted from each code – ranging from simple features such as density or complex features such as structure
   - We require the feature extraction be in the visualization tool; one for interactivity, and two, different simulations may have different feature extraction methods and thus are not comparable
2. Formulate/refine hypothesis about measurable differences between the codes
3. Test by Qualitative comparative visualization
4. Test by Quantitative comparative visualization

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Formulate/refine hypothesis

- Register the codes

1. Define and refine features
2. **Formulate/refine hypothesis about measurable differences between the codes**
   - Given the features defined in step one, the scientist makes a hypothesis about the simulation codes
3. Test by Qualitative comparative visualization
4. Test by Quantitative comparative visualization

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Qualitative comparative visualization

- Register the codes

1. Define and refine features
2. Formulate/refine hypothesis about measurable differences between the codes
3. **Test by Qualitative comparative visualization**
   - 3D visualizations are generated using the extracted features from the codes; they are visually compared to test the hypothesis
   - This is done through a visualization/small multiples spreadsheet
4. Test by Quantitative comparative visualization

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Quantitative comparative visualization

- Register the codes

1. Define and refine features
2. Formulate/refine hypothesis about measurable differences between the codes
3. Test by Qualitative comparative visualization
4. **Test by Quantitative comparative visualization**
   - Measured features are displayed in 2D quantitative plots for comparison to further test the hypothesis
   - The quantitative plots are combined with the 3D visualizations in the same visualization spreadsheet

- Go to step 1 or 2 until the codes are verified

Structured Comparative Visualization Process: Go to step 1 or 2 until the codes are verified

- Register the codes

1. Define and refine features
2. Formulate/refine hypothesis about measurable difference between the codes
3. Test by Qualitative comparative visualization
4. Test by Quantitative comparative visualization

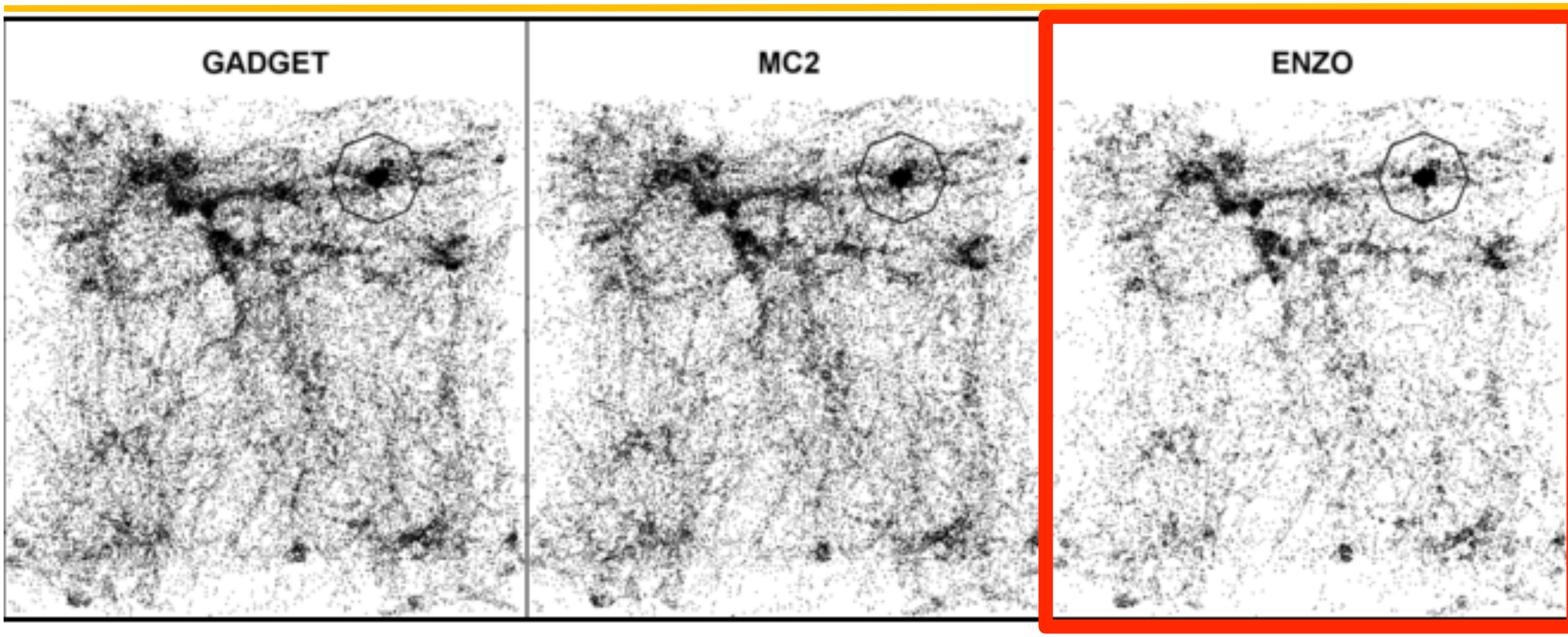
- **Go to step 1 or 2 until the codes are verified**
  - The process is repeated until the scientist is satisfied with the knowledge of the similarities or differences between the codes
  - This results in a final visualization, and a documented process from the steps taken
  - The document then can be used to disseminate scientific knowledge to the community

Case Study: Evolution of Halo Populations in AMR code

- **Halos are the one of the features cosmologists are most interested in**
  - Halos are bound clusters of points (dark matter)
- **AMR (adaptive mesh refinement) codes are popular for N-body cosmology simulations**
  - Computation time is saved by using low resolution meshes in low dense regions
  - AMR codes should have the same results as uniform grid codes, but faster
- **Run three codes and register their results**
  - 2 fixed resolution: GADGET-2 and MC^2
  - 1 AMR: Enzo – run at default mesh refinement settings

1. **Feature extraction – Halos and halo counts are derived from the data**
2. **Hypothesis A – An AMR code (Enzo) with peak resolution equivalent to a uniform grid code (GADGET-2 and MC^2) should resolve all halos of interest**

Step 3 and 4: Hypothesis A: Enzo should have as many halos as GADGET-2 and MC^2 – is false



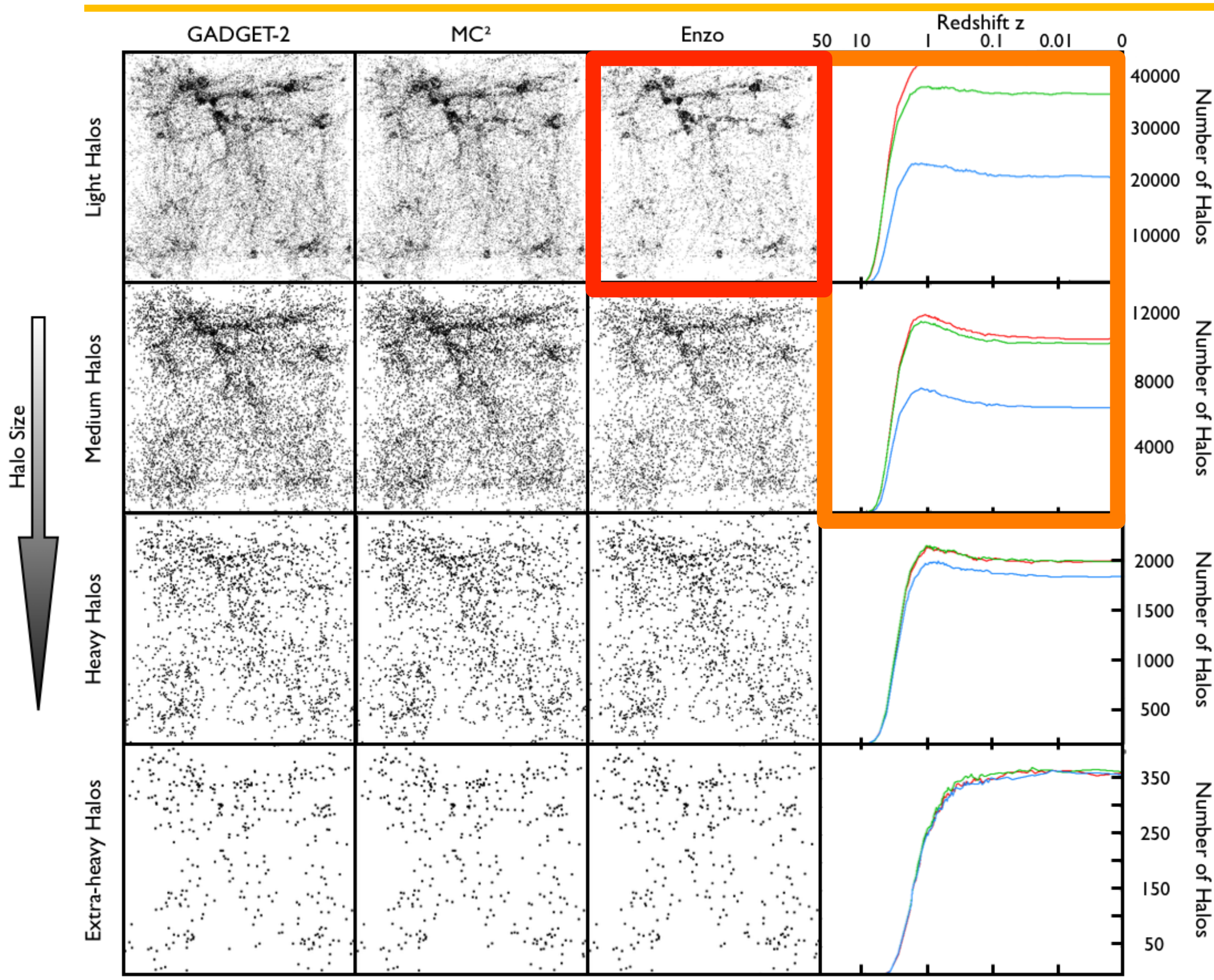
- **GADGET-2: 55512 halos, MC^2: 49293 halos, Enzo: 29099 halos**
- **Visually Enzo has far fewer halos, and this is supported by the quantitative halo count**

A New Hypothesis B

- **Hypothesis A was – An AMR code (Enzo) with peak resolution equivalent to a uniform grid code (GADGET-2 and MC^2) should resolve all halos of interest**
  - To understand why A is false, new hypotheses are offered
- **A new iteration of the workflow is started:**

1. **Feature Extraction – Halos are extracted, and their mass calculated**
2. **Hypothesis B – Halos do not form in early time steps and cannot be recovered**
   a) The halos in AMR codes do not form at early times, when the base resolution is still very low (density is low) and the halos cannot be recovered later
   b) Only halos of a certain size can be captured correctly, dictated by the base grid and not by the peak AMR resolution

Steps 3 and 4: Hypothesis B – Halos do not form early on in Enzo, and are not recovered – is supported



- **Enzo has far fewer light halos in the end time step and fewer medium halos**
- **Enzo (blue line in the graph) is not able to resolve light halos at the start, and is not able to recover the light halos over time**

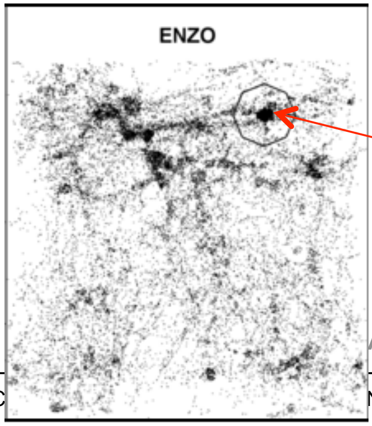
Discussion

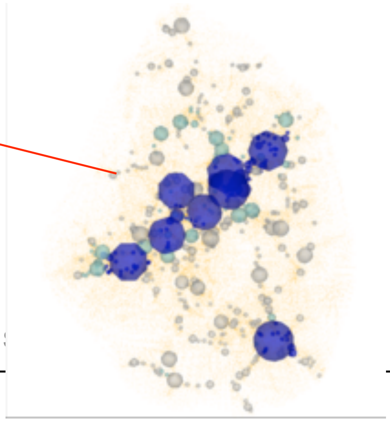
- **Verification of AMR codes is complete for what types of halos can be captured**
  - Enzo (at default refinement settings) is unable to capture light halos, and does not recover them over time
- **The structured visualization process achieved a scientific result, documentation, and reproducible results for scientists**
  - The hypothesis text and figures were provided for the Enzo scientific team to illustrate the issue of light halo formation with the default AMR refinement settings
- **The process requires interactive visualization, only the final results were shown here**
  - The search, iteration, and refinement is key to narrow results and test a hypothesis
  - The cosmologist was only able to find the results through repeated interactive visualization and iteration through the process
  - The 3D visualization was useful to give insight on where to direct the query and refine the hypothesis and visualization

Follow Up Case Study: Large Halo Formation Process

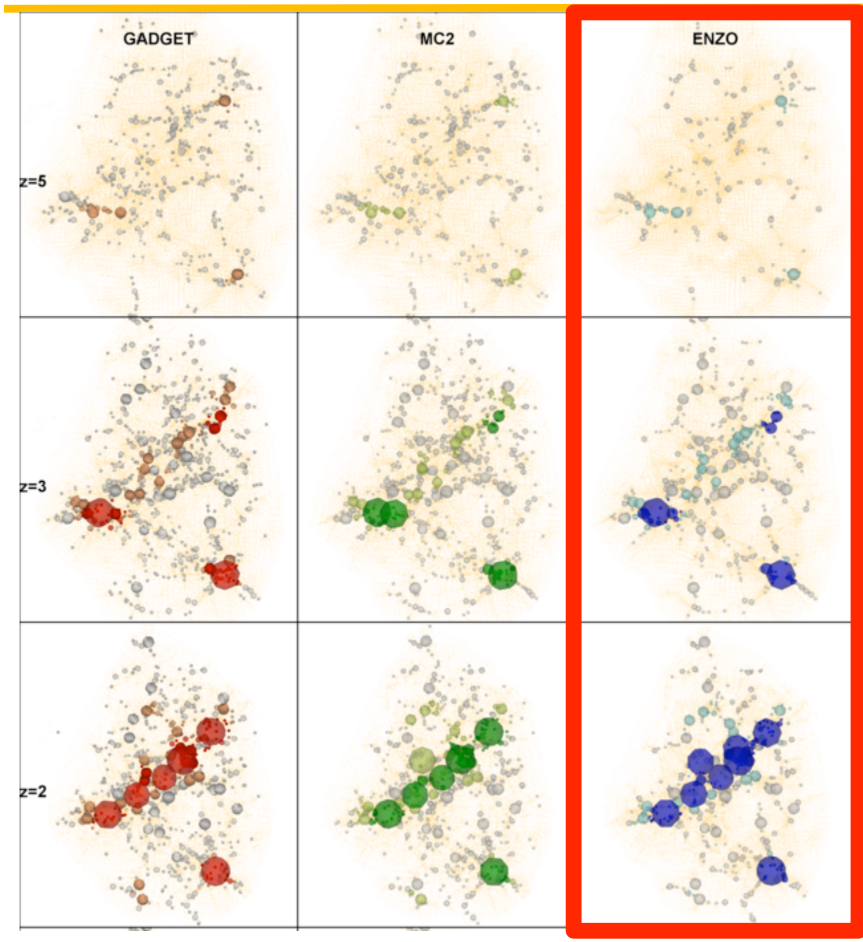
- **Are AMR codes able to resolve structures in extra-heavy halos, or will they be missing details due to low grid resolution at early time steps?**
  - Enzo has large halos and it might be possible that large halos are of high quality – they still able to have correct substructure
  - A particular halo is chosen (the third largest halo – Halo 3) and studied because of its large size and unusual shape (Halo 3 is elongated, normally halos are spherical)

1. **Feature extraction – Halo 3 and the subhalos that merge to form it are extracted, tracked, and the halo density is calculated**
2. **Hypothesis C – The AMR code should resolve substructures in a highly overdense regions reliably (regions of large halos)**



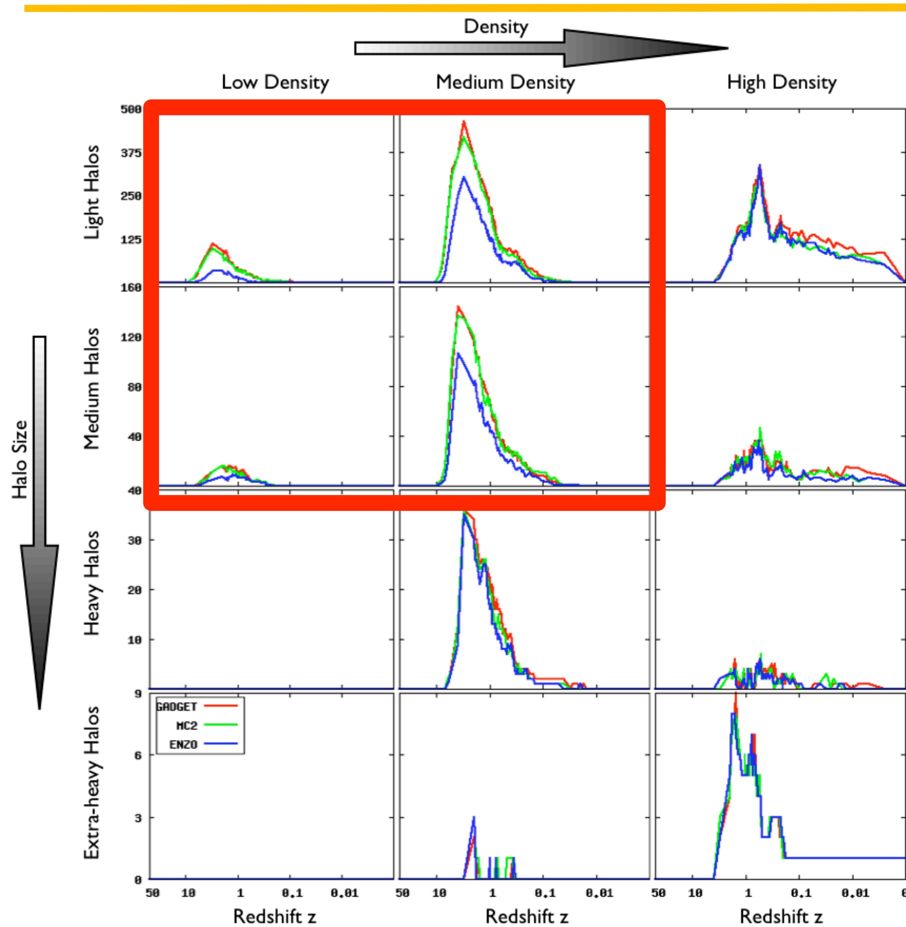


Step 3 – Hypothesis C – Halo 3 in Enzo has the same substructure as the others – appears to be false



- **In the final time step, the mass of Halo 3 is within a few percent in each simulation – Halo 3 in Enzo is the same size as the other simulations**
- **In an early time step, Halo 3 is missing light halos in Enzo (the gray dots, colored dots are large subhalos)**
- **The discrepancy seems to decrease over time, though the Enzo is still missing light halos (grey dots) in later time steps**

Step 4 – A New Hypothesis D – Enzo loses more light halos in low density regions – is supported, as well as C



- **All codes are able to resolve halos in high density regions**
  - Enzo is able to resolve heavy halos as well
- **Enzo is not able to resolve light and medium halos in all cases (in low and medium density regions)**
- **The light halo substructure of Halo 3 is lost, because they are not initially formed in light and medium density regions**

Discussion

- **From the analysis, AMR code cannot resolve small substructures even in extra-heavy halos**
  - As in the global case even for localized features, light and medium subhalos cannot be reliably resolved, even though Halo 3 had the same mass in AMR (Enzo) compared to GADGET-2 and MC^2
- **The results show that light and medium halos are lost in low dense regions for AMR**
  - The light and medium halos do not form in low and medium dense regions
  - They are not recovered over time, and therefore Enzo does not create the same substructure and formation history for Halo 3 compared the other simulations
  - Though, it does appear that AMR refinement does retain light and medium halos in highly dense regions

Final Words

- **From this visualization process the cosmologists were able to make a scientific discovery, and pass it on to the cosmology community**
  - The base grid needs to be fine enough to capture structure and features that evolve much later
  - The AMR refinement criteria needs to refine early enough to capture structure formation processes early – once halos are formed, it is too late
- **This process allowed the cosmologists to be more productive and achieve scientific results through visualization and analysis**
  - The structured step-by-step process makes it easy to follow and teach
  - It combines analysis, 3D, 2D, and quantitative visualization into a comparative visualization, rather than each being a separate task, to combine knowledge from each part and gain valuable insight
  - Interactivity was essential to go back to refine and reformulate the hypothesis
  - It provided a final result which is a reproducible document for scientific dissemination


Questions?