High-Performance Computing Applications in Cosmological Simulations

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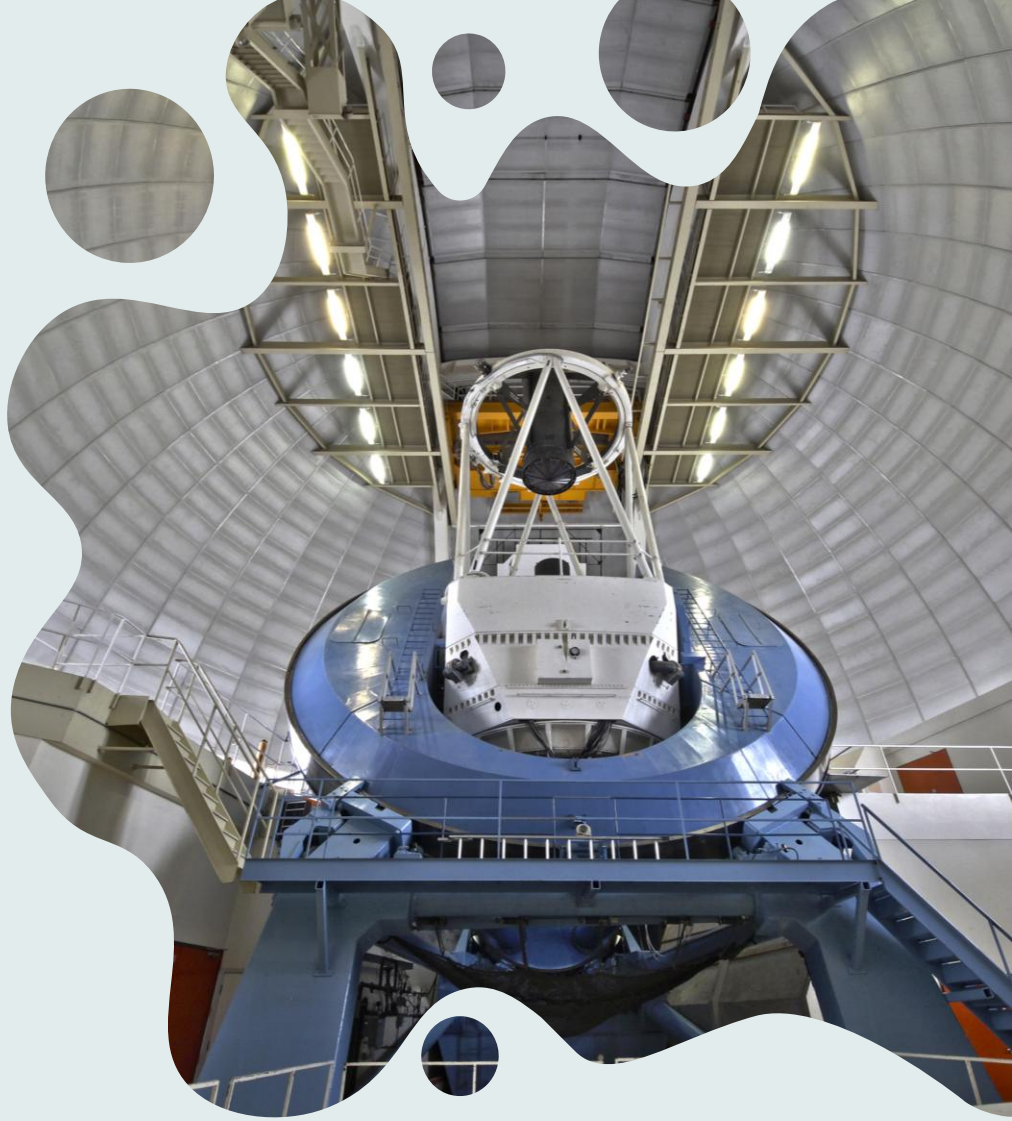
Why apply HPC to cosmological simulations?

- A cosmological simulation is a computer-based model that recreates and tracks the evolution of the universe over billions of years. e.g., simulating a star explosion evolution across 1 trillion particles.
- Too massive for traditional computing. For example, the IllustrisTNG simulation output was 128 TB large ~ 256 laptops
- Key needs: speed, memory, storage, real-time processing
- HPC to the rescue!
- Real world applications: Galaxy formation modeling, Processing cosmological survey results from the Large Synoptic Survey Telescope (LSST) and Dark Energy Spectroscopic Instrument (DESI)



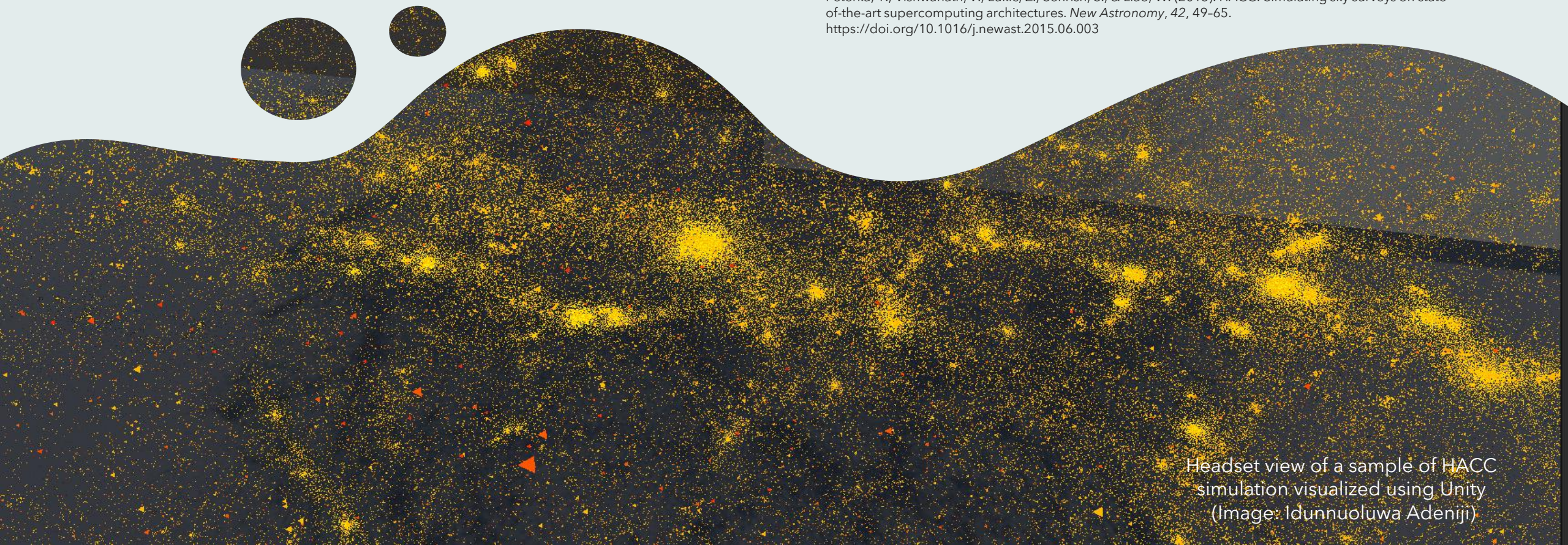
Dark Energy Spectroscopic Instrument (DESI)
Image: U.S. Department of Energy

Linke, L. (2020, May 28). *Speeding up cosmological simulations by zooming on what's important*. Astrobites. https://astrobites.org/2020/05/28/dynamicalzoomsimulations/

HARDWARE/HYBRID ACCELERATED COSMOLOGY CODE (HACC)

- A cosmology code for dark matter + structure formation
- Runs efficiently on CPUs, GPUs, and hybrid systems
- Scales to trillions of particles
- Projects: Outer Rim, Qcontinuum, Last Journey

Habib, S., Pope, A., Finkel, H., Frontiere, N., Heitmann, K., Daniel, D., Fasel, P., Morozov, V., Zagaris, G., Peterka, T., Vishwanath, V., Lukić, Z., Sehrish, S., & Liao, W. (2015). HACC: Simulating sky surveys on state-of-the-art supercomputing architectures. *New Astronomy*, *42*, 49–65. https://doi.org/10.1016/j.newast.2015.06.003



Headset view of a sample of HACC simulation visualized using Unity (Image: Idunnuoluwa Adeniji)

Supercomputing at work!

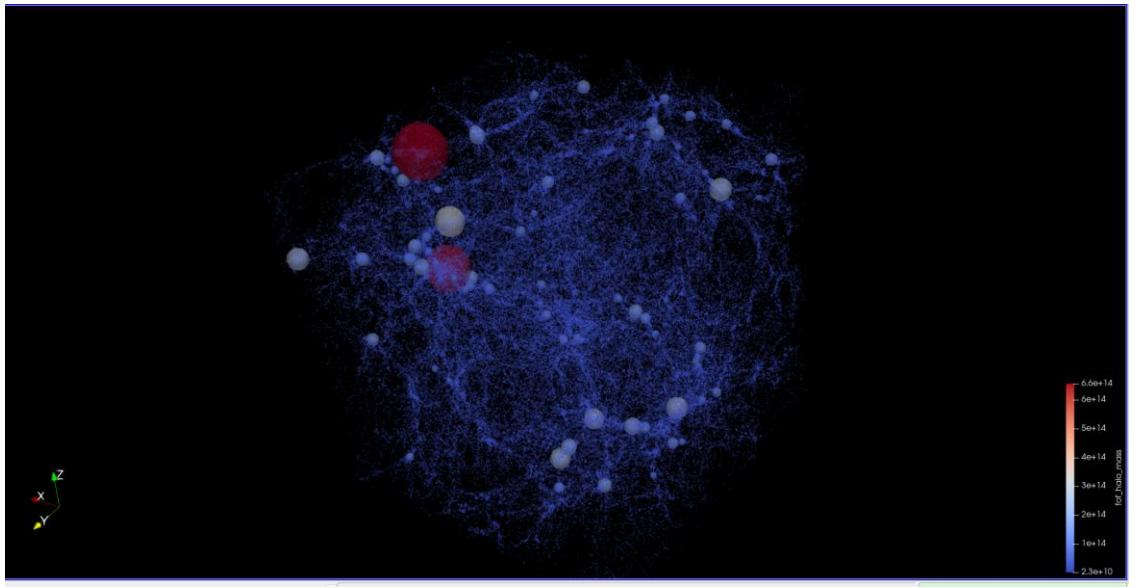
- Supercomputers: Polaris, Summit
- Data processing:
  - Parallel & Distributed computing
  - GPU acceleration
  - Extraction and filtration
- Performance: Years → days of simulation.

Polaris supercomputer at the Argonne Leadership Computing Facility (Image: Argonne National Laboratory)

Habib, S., Pope, A., Finkel, H., Frontiere, N., Heitmann, K., Daniel, D., Fasel, P., Morozov, V., Zagaris, G., Peterka, T., Vishwanath, V., Lukić, Z., Sehrish, S., & Liao, W. (2015). HACC: Simulating sky surveys on state-of-the-art supercomputing architectures. New Astronomy, 42, 49–65. https://doi.org/10.1016/j.newast.2015.06.003

In Situ Visualization with ParaView

- Challenge: Huge data output (petabytes)
- Solution: Visualize during runtime using ParaView + Catalyst (This connects simulation output directly to the rendering engine)
- Enables real-time adjustments



Post-processing visualization of HACC dataset in ParaView
(Image: Idunnuoluwa Adeniji)

Adamo, J., Emberson, J. D., Brooks, E., Rizzi, S., Insley, J., & Papka, M. E. (2018). Exploring Visualization Techniques with HACC Simulation Data. Conference: LDAV, 92–93. https://doi.org/10.1109/ldav.2018.8739228

Challenges

Computational cost and energy consumption

Data management and transfer

Software scalability to exascale systems

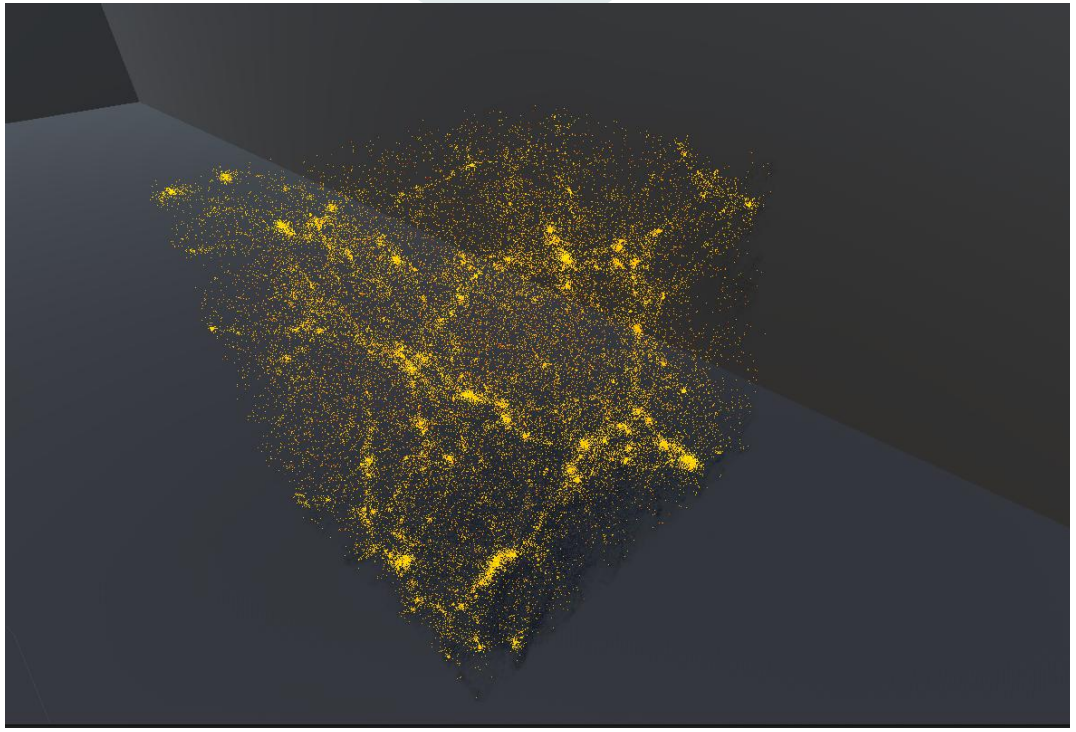
Cognitive and usability limits in data interaction

Taking HACC into the Exascale Era: New Code Capabilities, and Challenges. (2024, February 28). IDEAS Productivity. https://ideas-productivity.org/events/hpcbp-079-hacc

Future Directions

- Integrating Artificial Intelligence to enhance pattern recognition in large cosmological datasets.
- Accelerating simulation runtimes through optimized algorithms and hardware advancements.
- Advancing Human-Computer Interaction (HCI) to support more intuitive and immersive data exploration in VR/AR environments.
- Establishing direct Unity integration for seamless in situ visualization and real-time interaction during simulations.

Adeniji, I. A., Insley, J. A., Joiner, D., Mateevitsi, V. A., Papka, M. E., & Rizzi, S. (2024). Exploring Large-Scale Scientific Data in Virtual Reality. Conference: LDAV, 75–76. https://doi.org/10.1109/ldav64567.2024.00019



3D visualization of a HACC cosmological dataset rendered in Unity for immersive exploration.
Image: Idunnuoluwa Adeniji

Conclusion

Question
Comments
Concerns