SIGHT

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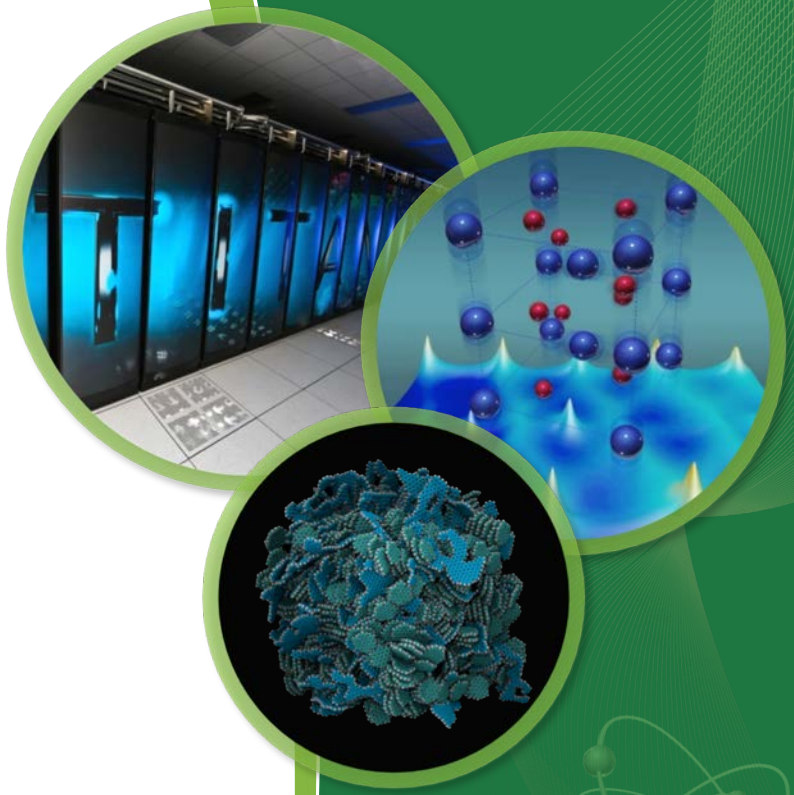

Collaborators

Aaron Knoll, Peter Messmer (NVIDIA Viz Team)
Dylan Lacewell (NVIDIA Optix Team)

ORNL is managed by UT-Battelle
for the US Department of Energy

This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

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Introduction

- Scientific visualization is one of the components to enable scientific discovery through visual imaginary of computer simulations.
  - Batch based visualization
  - In-situ visualization
  - Exploratory Visualization

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Introduction

- According to my experience with current users, I found traditional visualization tools can overwhelm them for some tasks, sometimes we just want:
  - To viz. their dataset, with no hassle, to see what a simulation produced, or for model preparation.
  - Explore their datasets from different camera views.
  - Explore their dataset to see what transition function works best.
  - Cut their dataset to generate transversal views.
- And what about…
  - producing nice images for your Journal covers or for the OLCF site?
  - Make easier PhD students life…
- **Accelerate your visualization pipeline with real-time feedback**

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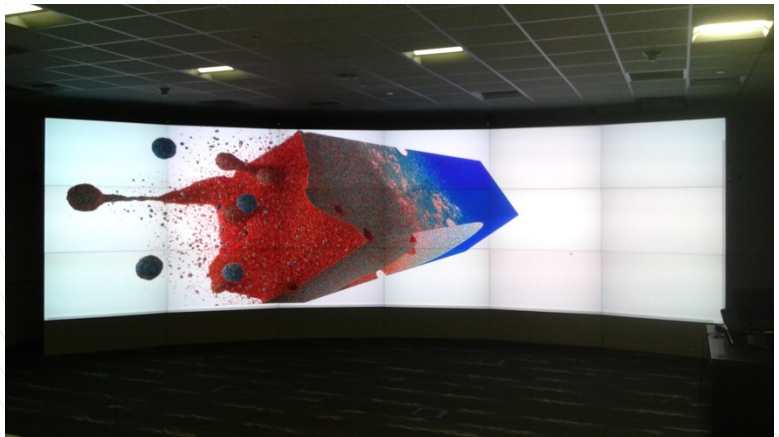
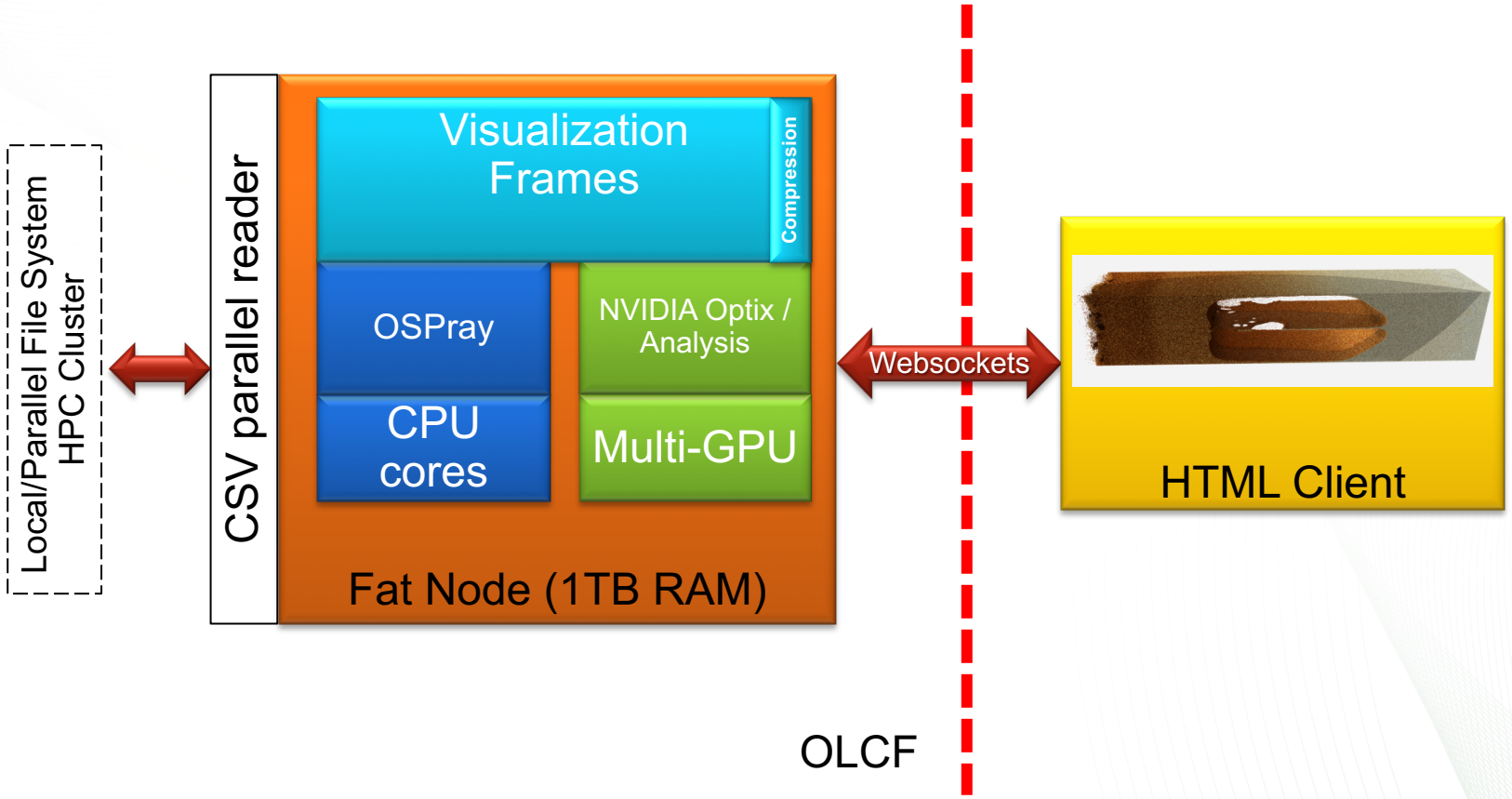
SIGHT:
Exploratory Visualization of Scientific Data

- Lightweight tool
  - Load your data
  - Perform exploratory analysis
  - Visualize/Save results
- Heterogeneous scientific visualization
  - Advanced shading to enable new insights into data exploration.
  - Multicore and manycore support.
- Remote visualization
  - Server/Client architecture to provide high end visualization in laptops, desktops, and powerwalls.
- Parallel I/O
- Supports interactive/batch visualization
  - In-situ (some effort)
- Designed having OLCF infrastructure in mind.



Current SIGHT System Architecture



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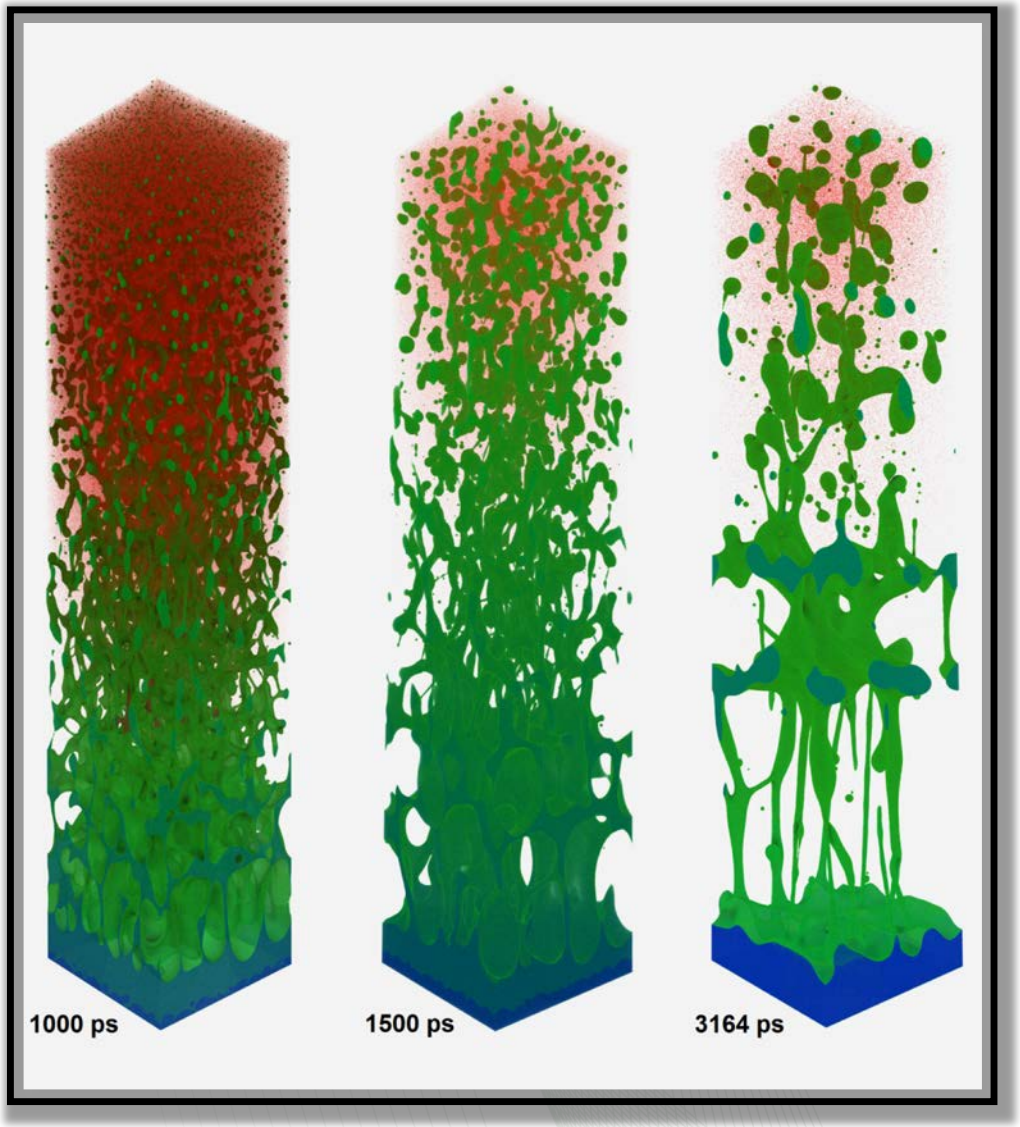
Current Users

- INCITE MAT 130 "*Petascale simulations of short pulse laser interaction with metals*" PI Leonid Zhigilei, University of Virginia

"Large-scale atomistic simulations of laser interactions with metal targets are used to:

- Elucidate the mechanisms of generation of Laser Induced Periodic Surface Structures in the regime of strong ablation
- Reveal the initial dynamic interaction between ablation plume and liquid environment leading to surface morphology modification and nanoparticle generation in pulsed laser ablation in liquids

Computational predictions have direct **impact** on interpretation of experimental observations and design of new laser processing technologies."



M. V. Shugaev, C. Wu, O. Armbruster, A. Naghilou, N. Brouwer, D. S. Ivanov, T. J.-Y. Derrien, N. M. Bulgakova, W. Kautek, B. Rethfeld, and L. V. Zhigilei, Fundamentals of ultrafast laser-material interaction, *MRS Bull.* **41** (12), 960-968, 2016.

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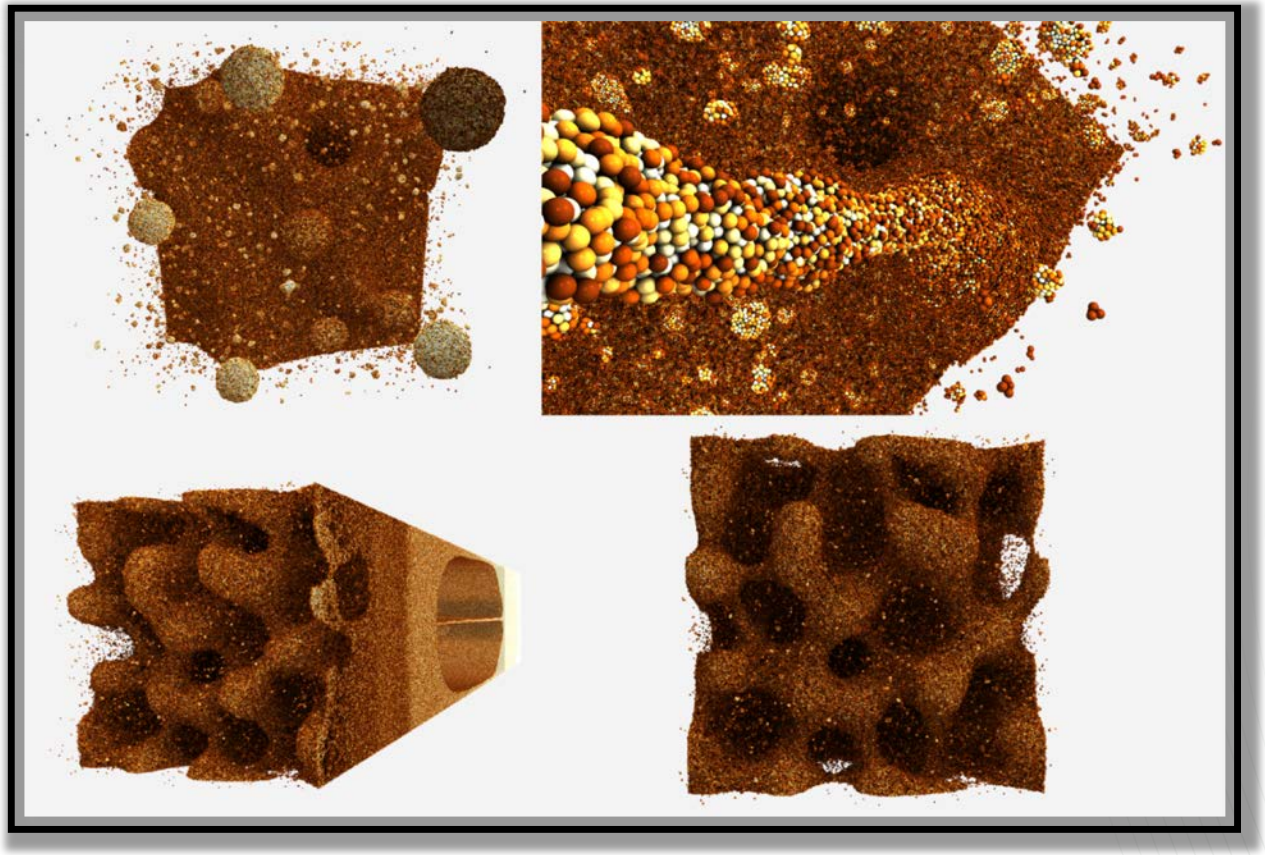
Laser ablation in liquid environment



C.-Y. Shih, M. V. Shugaev, C. Wu, and L. V. Zhigilei, Generation of subsurface voids, incubation effect, and formation of nanoparticles in short pulse laser interactions with bulk metal targets in liquid: Molecular dynamics study, *J. Phys. Chem. C* **121**, 16549-16567, 2017.

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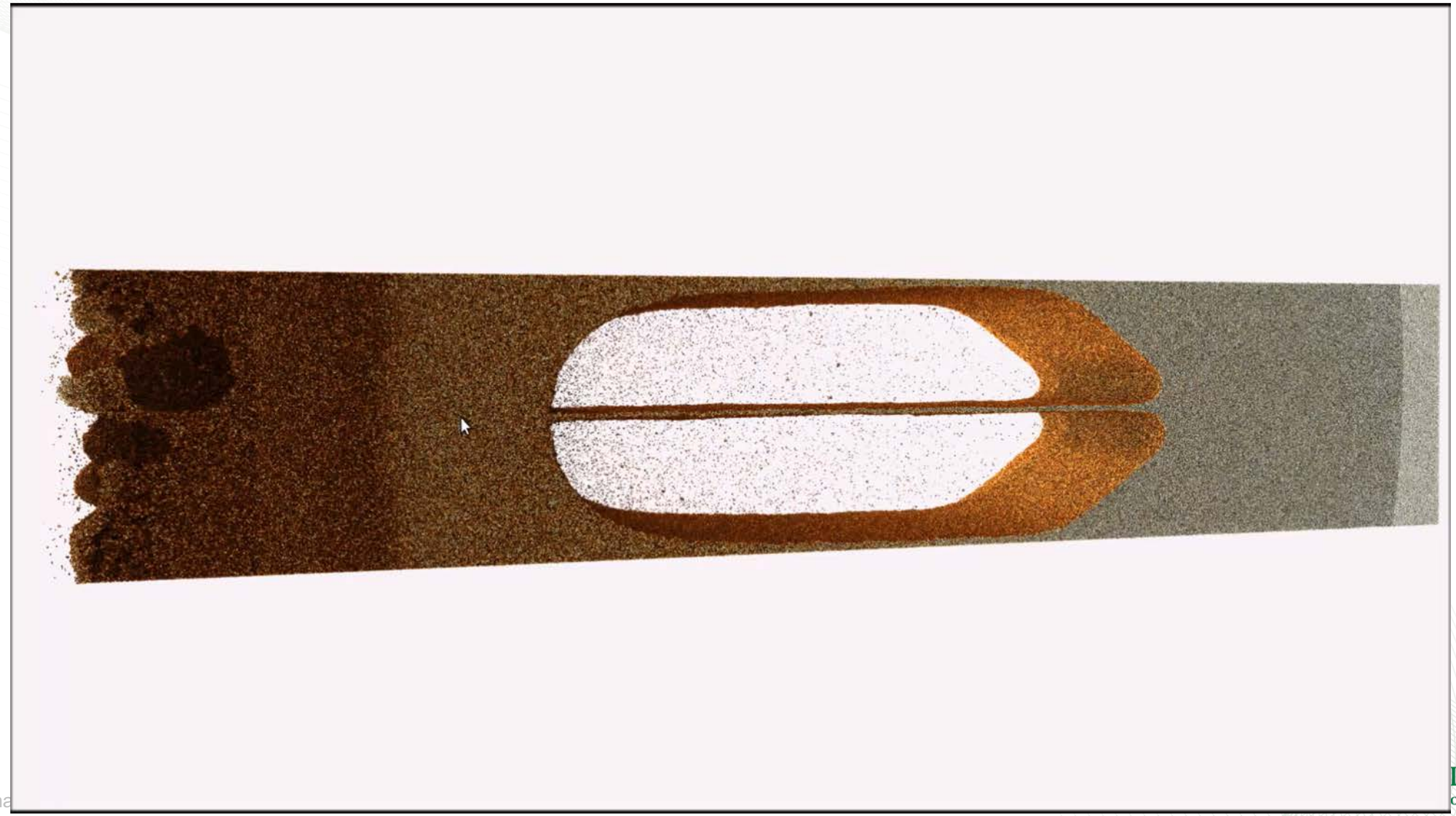

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To appear in Nanoscale 18, and as seen in:

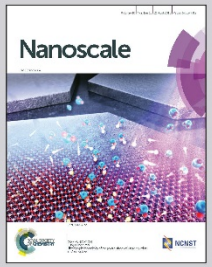
C.-Y. Shih, R. Streubel, J. Heberle, A. Letzel, M. V. Shugaev, C. Wu, M. Schmidt, B. Gökce, S. Barcikowski, and L. V. Zhigilei, Two mechanisms of nanoparticle generation in picosecond laser ablation in liquids: the origin of the bimodal size distribution, *Nanoscale* **10**, 6900-6910, 2018.

Showcasing collaborative research from University of Virginia, USA and University of Duisburg-Essen, Germany.

Two mechanisms of nanoparticle generation in picosecond laser ablation in liquids: the origin of the bimodal size distribution

This image illustrates two mechanisms of nanoparticle generation in picosecond laser ablation of metal targets in liquids revealed in large-scale atomistic simulations: rapid nucleation and growth of small nanoparticles in an expanding metal-liquid mixing region, proceeding simultaneously with hydrodynamic instabilities that launch large liquid droplets into dense and cold liquid environment. The computational predictions are supported by single and double pulse experiments showing the emergence and optical activation of small satellite microbubbles surrounding the main cavitation bubble generated in laser ablation.

As featured in:



See Bilal Gökce, Leonid V. Zhigilei *et al.*, *Nanoscale*, 2018, **10**, 6900.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/nanoscale

Registered charity number: 207890

Current Users

INCITE BIP115 PI “All-atom Simulations of Photosynthetic and Respiratory Energy Conversion” PI Abhishek Singharoy, Arizona State University

- Pre-visualization of digital reconstruction of the Terazaki Ramp (Noah Trebesch & Emad Tajkhorshid)
  - It is a part of The endoplasmic reticulum (ER) and serves multiple functions, being important particularly in the synthesis, folding, modification, and transport of proteins
- Around 4 billion atoms

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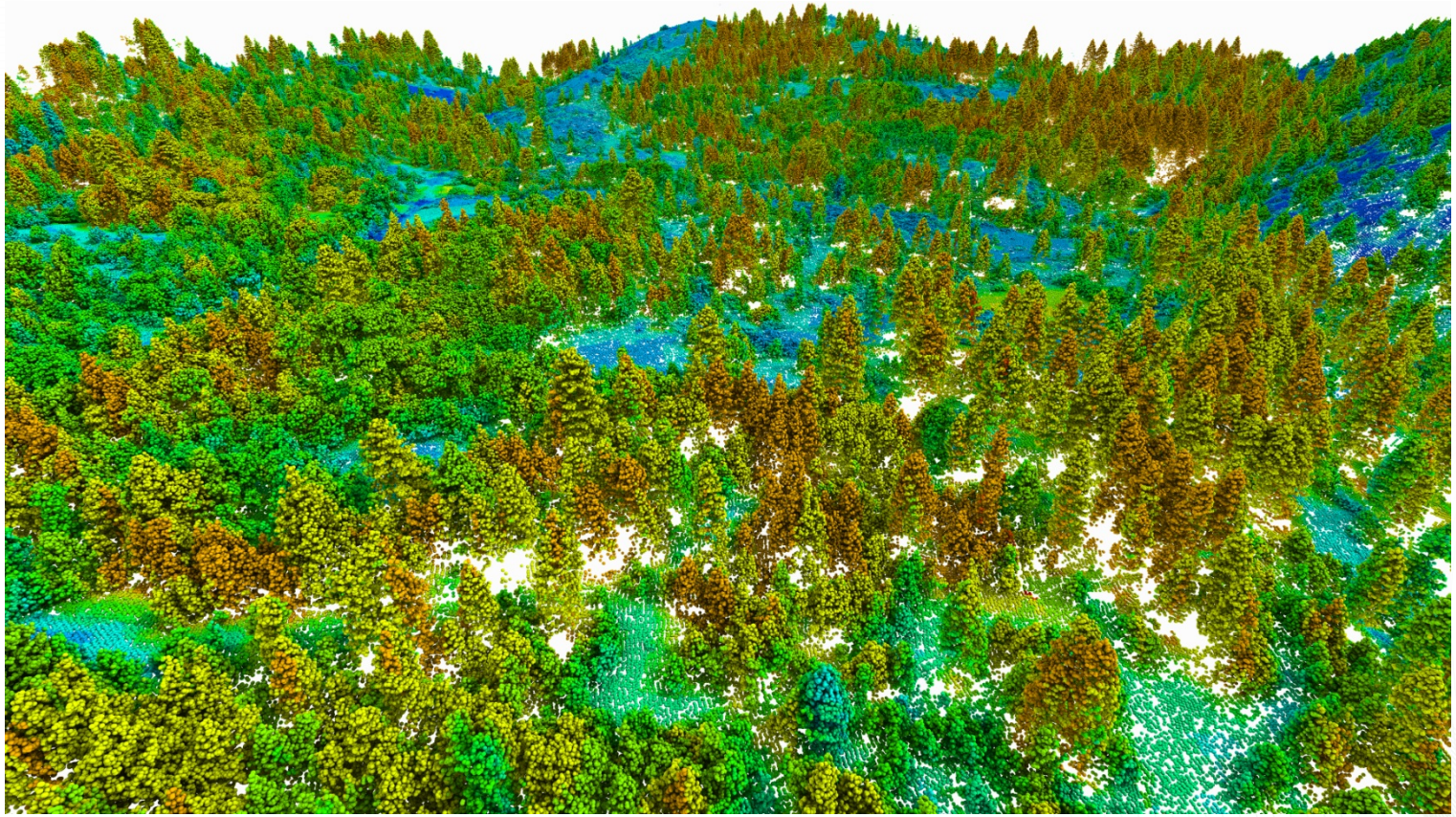
Current Users

DD GEO126 The Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC) Data Visualization



Close up to 4 Billion could point LiDAR data

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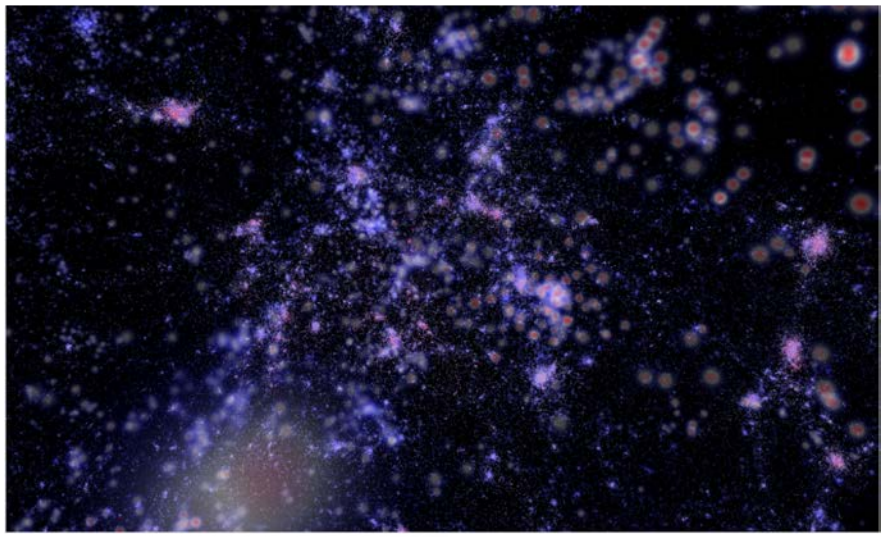
Final Remarks

- SIGHT uses cases are for atomistic simulations however it can be extended according to your needs to support:
  - Meshes, streamlines, volumes (structured, Unstructured and AMR)
  - RBF volumes (Aaron Knoll NVIDIA)
- SIGHT does not seek to substitute your viz tool, it is a complement.
- SIGHT is not just a tool is an OLCF custom service.
- Working with NVIDIA to bring SIGHT into SUMMIT

2014 Dark Sky cosmology simulation
Credit Aaron Knoll NVIDIA



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