SIGHT

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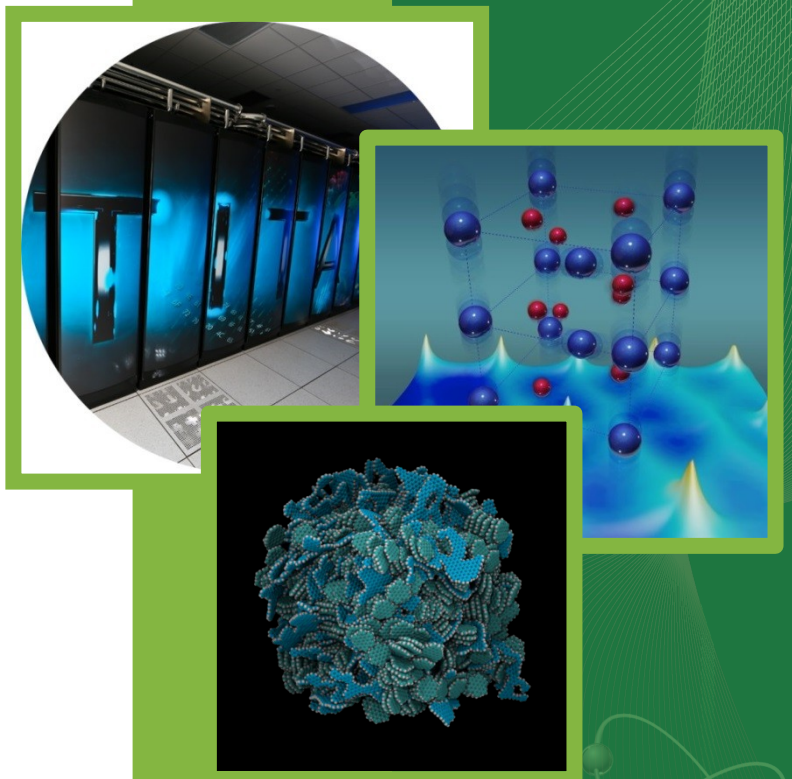


This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

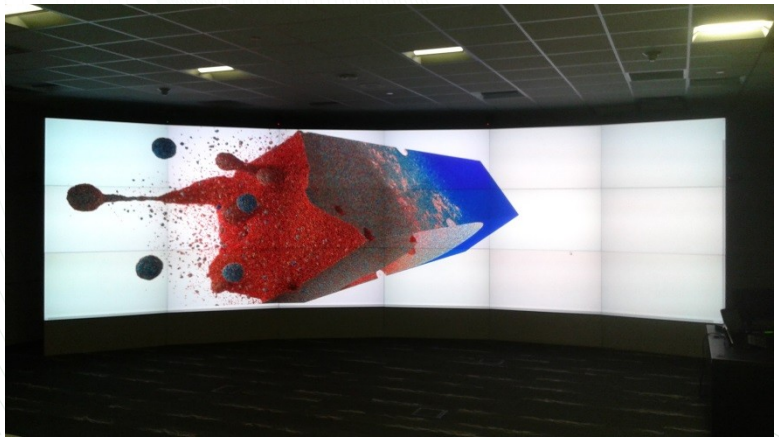
Introduction

Sight is an exploratory visualization tool for large scale datasets supporting manycore and multicore advanced shading, remote and interactive scientific visualization, parallel I/O and large scale displays. Sight is currently deployed in the OLCF systems to support TITAN's users in their visualization and analysis tasks.

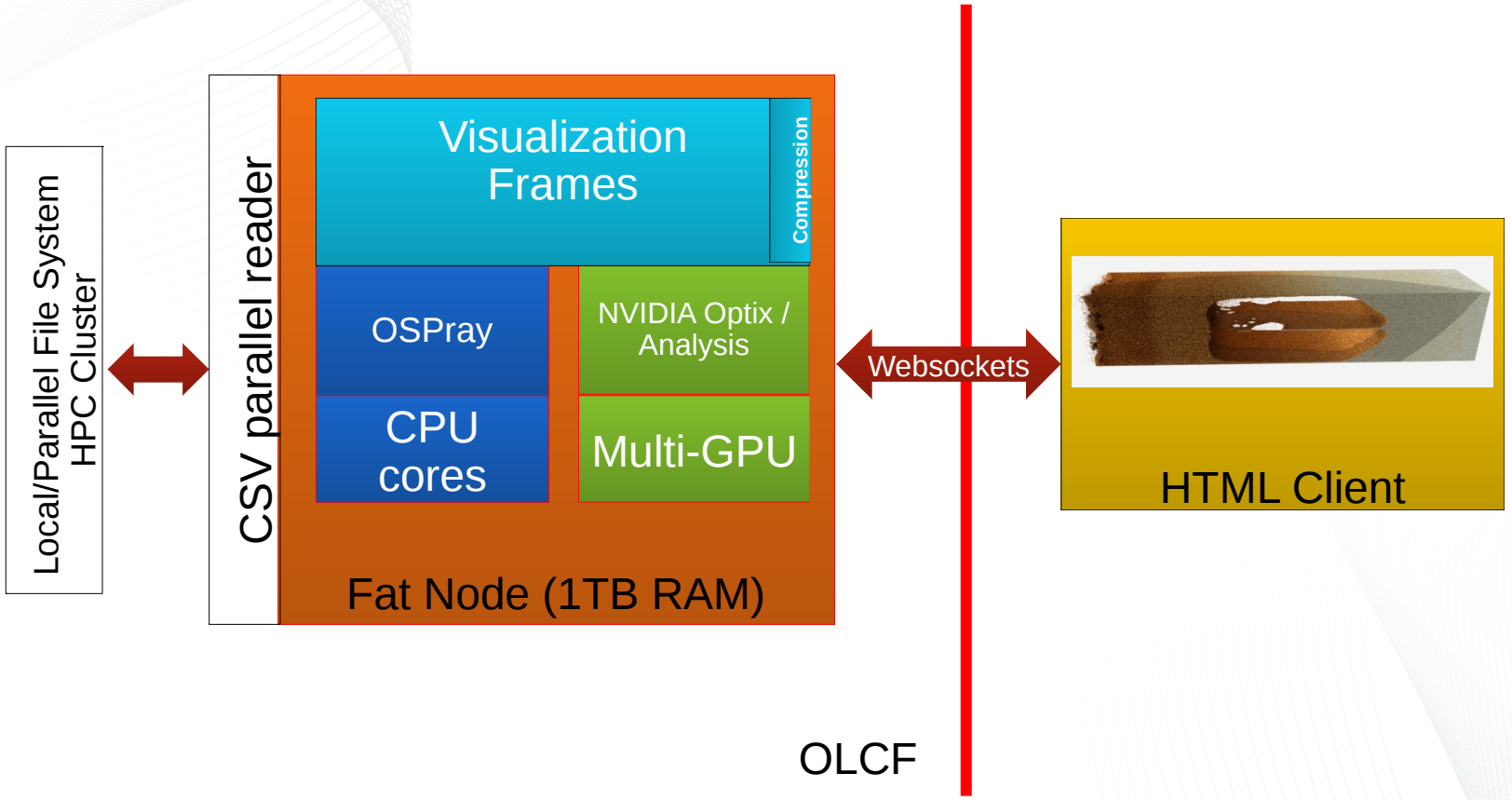
- **Accelerate your visualization pipeline with real-time feedback**

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



Achievements

- Extending and scale Sight to support bigger datasets coming from SUMMIT and support multiple time steps of significant size.
- Three strategies discussed:
  - Sort last compositing included (and improved) in OSPRay
  - Sort last compositing based on TOD-Three algorithm (Pascal Grosset LANL)
  - GraviT (Paul Navratil TACC)
- SIGHT deployment in ALCF systems.
  - Several ALCF users working on material science.
- Discussions with Dave DeMarle to deploy Paraview in SUMMIT

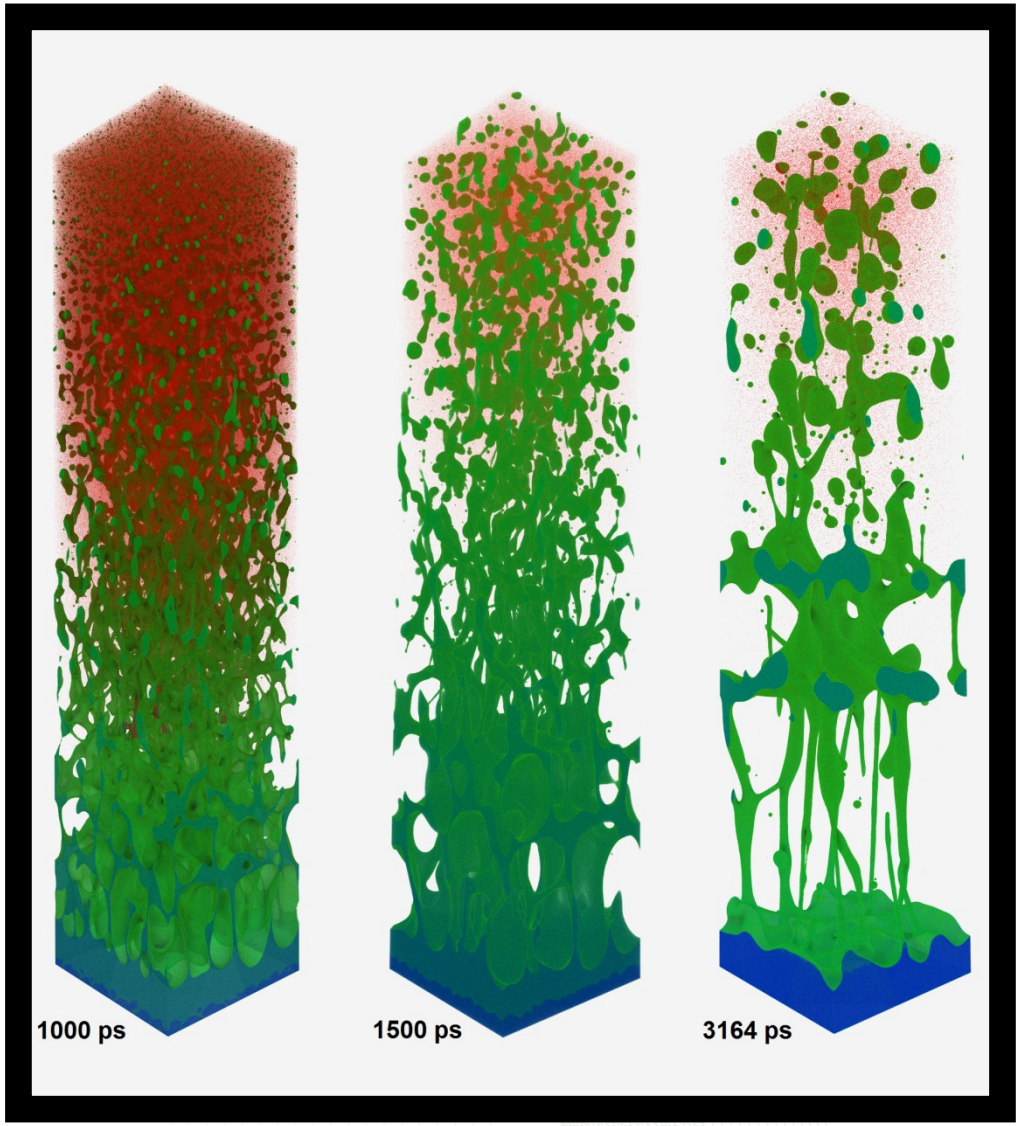
Current Users
Viz. using OSPray backend

- 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."



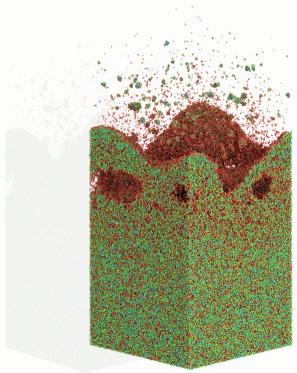
M. V. Shugaev, C. Wu, O. Armbruster, A. Naghilou, N. Brouwer, D. S. Ivanov, T. J.-Y. Derrien, N. M. Bulgakova, W. Kautek, B. Rethfeld, and L. V. Zhigilei, Fundamentals of ultrafast laser-material interaction, *MRS Bull.* **41** (12), 960-968, 2016.

Current Users

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

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.

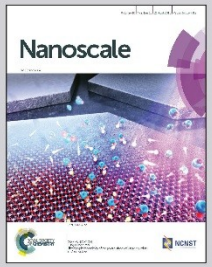


Showcasing collaborative research from University of Virginia, USA and University of Duisburg-Essen, Germany.

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

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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