Computing Grand Challenge Program for Open Science

Advancing science on Top500-rated machines on the unclassified network

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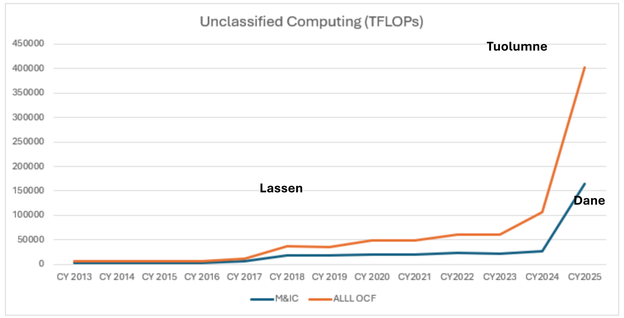
For 20 years, LLNL's Computing Grand Challenge (GC) Program has allocated significant computational resources to LLNL Principal Investigators and their teams to perform cutting-edge research. The 2025 program awarded more than 5 million node hours (61.229 sustained petaflops) to projects that address compelling, large-scale problems and advance science.

Funding: LC receives $11M–16M/year for staff and hardware to support unclassified computing.

Principal Investigators Compete for GC Awards

Tier 1 awardees receive up to 200K node hours on the Advanced Technology Systems (Tuolumne and Lassen) and the Commodity Clusters (Dane and Ruby). The collective peak performance of the LC machines on the unclassified network has increased at an incredible rate by tracking the Advanced Simulation and Computing platforms. Tier 2 awardees receive 25–50K node hours.



PIs Have Access to Multiple Top500 Machines

TUOLUMNE 288.0 PF

LASSEN 18.2 PF

DANE 7.0 PF

RUBY 3.7 PF

Project Selection: A Competitive Process

Grand Challenge allocations are awarded once a year, following a formal, competitive proposal and review process based on the several review factors:

- Significance and impact of science
- Significance and impact of computational approach
- Quality of HPC research plan
- Quality/extent of external collaborations
- Alignment with Laboratory S&T strategic vision
- Past Grand Challenge performance

Existing projects must resubmit each year to continue their access.

Computing resources are the enabler; project success relies on the strength of researchers' ideas.

Publications, Results, Presentations

Grand Challenge recipients have reported more than 190 key publications and invited talks.

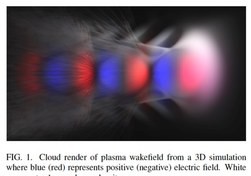
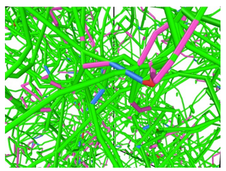
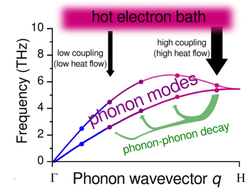


FIG. 1. Cload render of plasma wakefield from a 3D simulation where blue (red) represents positive (negative) electric field. White represents plasma charge density.



Dislocation Dynamics



Select seminar abstracts and visualizations from publications.

Representative publications:

Bertin, N., Bulatov, V.V., and Zhou, Z. (2024). "Learning Dislocation Dynamics Mobility Laws from Large-Scale MD Simulations." *Computational Materials,* 10, 192. doi: 10.1038/s41524-024-01378-4

Borges-Araújo, L., Borges-Araújo, A., Ozturk, T.N., et al. (2023). "Martini 3 Coarse-Grained Force Field for Cholesterol." *J. Chemical Theory and Computation,* 19(20), 7387–7404. doi: 10.1021/acs.jctc.3c00547

Appelquist, T., Brower, R.C., Cushman, K.K., et al. (2023). "Hidden Conformal Symmetry from the Lattice." *Physical Review D,* 108(9). doi: 10.1103/PhysRevD.108.L091505

Pateloudis, S., Bergner, G., Hanada, M., et al. (2023). "Precision Test of Gauge/Gravity Duality in D0-Brane Matrix Model at Low Temperature." *Journal of High Energy Physics,* 2023(71). doi: 10.1007/JHEP03(2023)071

Two Levels of Allocation

CY25 Tier 1: Highest visibility and impact, allocations of 100k–200k node hours

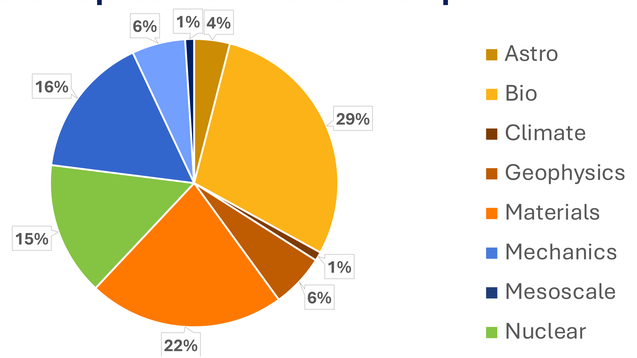
PI	Topic
Bertin	Unraveling dislocation multiplication with molecular dynamics simulations
Carpenter	Ft pathogen countermeasure design using machine learning and membrane modeling
Kravvaris	Computing atomic nuclei exploring the universe through a nuclear lens
McGill	The next generation of exoplanet atmospheric models for the James Webb space telescope and beyond
Vranas	Strongly interacting composite particle scattering with machine learning

CY25 Tier 2 (summarized, 17 total awards): High visibility and impact, allocations of 25k–50k node hours

Discipline	Research topic summary
Mechanics	Bio and chemical weapons countermeasures
Materials	Studies using laser-induced non-equilibrium conditions; cracking in additive manufactured tungsten; oxidative stability of polymers
High-energy-density plasmas	Kinetics in HED plasmas with deep learning
Bio	Computing-aided drug discovery; vascular digital twins for medical diagnoses ★
Geophysics	Seismic code improvements and simulation of seismic sources for hazard assessment ★
Molecular dynamics	Advancing nanostructured electrocatalysts through ML-enhanced MD ★
Astrophysics	High-fidelity fission simulations for astrophysics

★ See ERC poster on this topic

Projects Represent Diverse Disciplines



Allocation recipients' project disciplines from 2020–2025 (102 projects).

Lawrence Livermore National Laboratory

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NNSA National Nuclear Security Administration