High-Performance Computing and Software Sustainability: Toward Green Software Development

Antigoni Georgiadou, Ph.D. Oak Ridge National Laboratory

Webinar Series: HPC Best Practices Webinars

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

Green Software

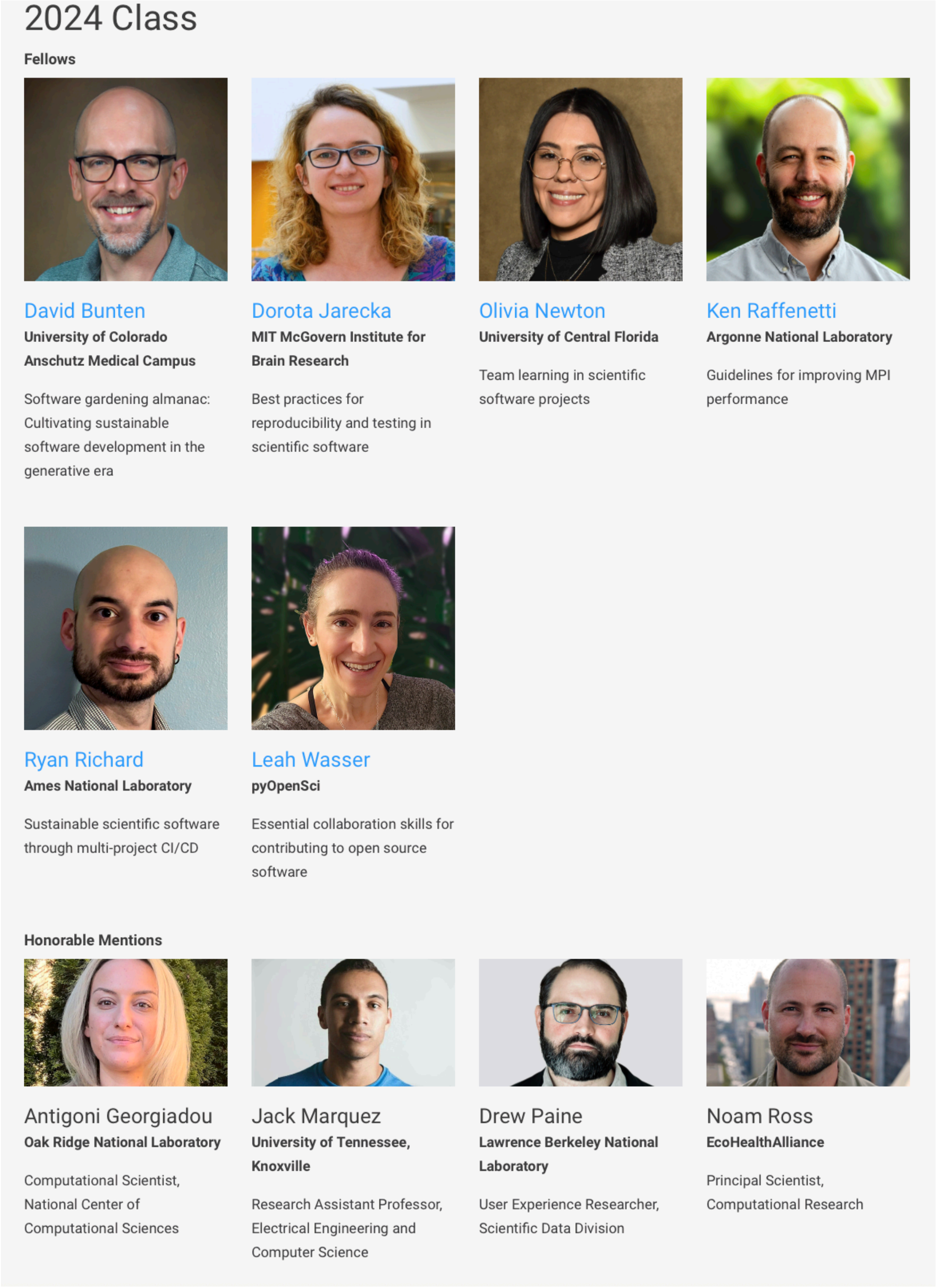
- Scientific **applications** rely on robust & efficient software
- Software will not consume energy but can **indirectly** influence operations within computational resources contributing to carbon emissions and energy consumption
- Like computer **hardware**, software is part of the problem for environmental sustainability
- Software **practices** will be one of the aspects to be considered for future planning in the HPC regime

Within this framework I will discuss current and future work on enabling a somewhat green software philosophy

Antigoni Georgiadou, PhD- 2024 BSSw Award

- Background with respect to the computational and outreach aspect
  - Computational Scientist in Mathematics at the Oak Ridge National Laboratory & a member of the Algorithms & Performance Analysis Group in the Science Engagement Section (Lead- Dr. Phillip C. Roth, ORNL)
  - Part of the FLASH-X **astrophysics** collaboration (Dr. Bronson Messer, ORNL) & liaison of the HACC team to perform cosmology simulations (Dr. Salman Habib & Dr. Katrin Heitmann, ANL)
  - Been serving as the OLCF liaison for the XGC **fusion** collaboration (PI- Dr. CS Chang, PPPL)
  - Collaborate with the Randle's Lab at Duke (PI- Dr. Amanda Randles, Duke University)
  - Technical Committee member of **INCITS for Fortran** and the parent Programming Languages (PL22). The technical committee works on the interpretations of the current standard for Fortran and develops the list of new features for the following revisions (Committee Lead- Dr. Reuben Budiardja, ORNL)
  - Accelerated Data Analytics and Computing Institute (**ADAC**) Executive Committee Director (Dr. Tjerk Straatsma, ORNL)
  - Chair of the workshop on Enabling Predictive Science with Optimization and **Uncertainty Quantification** on HPC (EPSOUQ-HPC) at the SC23 & SC24 (Co-chair Dr. Tiernan Casey, SNL)

- BSSw Fellowship Scope
  - Raise awareness of good software practices, improve scientific productivity, and inform for ongoing efforts for sustainability planning.
- Papers
  - "Uncertainty-Informed Approximate Computing for Energy-Efficient Visualization of Large-Scale Data", Athawale T. et al., ASCR EECS Workshop
  - "Towards Sustainable Supercomputing", Shin W. et al., paper accepted at the Sustainable Supercomputing workshop (SusSup24) at SC24



BSSw Scope for "Green software"

better scientific software

https://bssw.io/

- Build community
- Have open conversations
- Getting feedback
- Training & incremental improvement of best practices
- Vision going forward: opportunity to discuss supporting and sustaining software
- Outreach to the community

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- **Logistics: interested in suggestions for ways to access a media room with support for audio and optical/recording infrastructure (keeping in mind that this is not a funded project).**
- **Suggestions for speakers that could be a good match as guests, familiar on the topic, etc.**

Energy efficiency is especially critical at ORNL

OAK RIDGE National Laboratory

Science Areas Work With Us Abo

News

Plant CO2 uptake rises by nearly one third in new global estimates

October 21, 2024

An observation tower overlooks a Panamanian rainforest where scientists from ORNL and other partners are working on the DOE Next Generation Ecosystem Experiments Tropics project, gathering ground measurements that are used to analyze tropical forest carbon cycling. Credit: Jeff Warren/ORNL, U.S. Dept. of Energy

RESEARCHERS

Lianhong Gu

Organizations

- Biological and Environmental Systems Sci Directorate
- Environmental Sciences Division
- Earth Systems Science Section
- Ecosystem Processes Group
- Climate Change Science Institute

Related News

- Climate Change
- Decarbonization
- Environment

OAK RIDGE National Laboratory

Researchers turn coal into graphite for clean energy, electric vehicle batteries

Science Areas

December 12, 2024

Credit: ORNL, U.S. Dept. of Energy

Yesterday's polluting fuel could be transformed into a valuable material for tomorrow's electric vehicle batteries, thanks to a wide-ranging research project that utilizes expertise spanning the Department of Energy's Oak Ridge National Laboratory.

ORNL researchers created and tested two methods for transforming coal into the scarce mineral graphite, which is used in batteries for electric vehicles and renewable energy storage.

https://www.ornl.gov/news/two-paths-many-benefits

Supercomputers & Energy- TOP500 & GREEN500

- ***Greenness*** is a constraint that should be optimized to enhance power measurement methodology
- A typical supercomputer will consume electrical energy that converts into heat that requires cooling to be processed.
- Ranking of systems that occurs twice a year with a power measurement methodology
- Metrics:
    - Flops/Watt
    - High-performance LINPACK (HPL)
    - Levels of power measurement: L1/L2/L3-> range from average power to energy consumed
- Rmax - Maximal LINPACK performance achieved
- Rpeak - Theoretical peak performance

Ranked No1 in the TOP500 list Jun22-Nov22-Jun23-Nov23-Jun24

Frontier debuted as No1 in the TOP500 list and its TDS system reached No2 on the GREEN500 list the same year

URL: https://www.top500.org/

On the software side

*Power consumption of data and HPC centers is gradually becoming a hot topic given the growth of **AI and exascale systems** are requiring 30+ MW, enough to power sizable towns. There is a universal effort towards **green software development** with academia, government, and industry spearheading the discussion on how software developers will produce **better software** in terms of **more energy efficient approaches**.*

What makes software cost efficient?

- Achieve desired science results while minimizing time of execution for given tools and architectures
  - Optimized modular design
  - Open source technologies/well tested and widely used
  - Code optimization
  - Automation for repetitive tasks
  - CI for automated build/testing/feedback loops to eliminate blind spots

Visualization and Energy Efficiency for Large Data

2024 Energy-Efficient Computing for Science Workshop

Sponsored by the U.S. Department of Energy,
Office of Advanced Scientific Computing Research (ASCR)
September 9-12, 2024
Bethesda, MD

- Position Paper on **Uncertainty-Informed Approximate Computing for Energy-Efficient Visualization of Large Data**T. M. Athawale, D. Pugmire, C. R. Johnson, K. Moreland, P. Rosen, A. Georgiadou, T. Beck

  [Paper] U.S. Department of Energy's ASCR Workshop on Energy-Efficient Computing for Science, Bethesda, MD, 2024

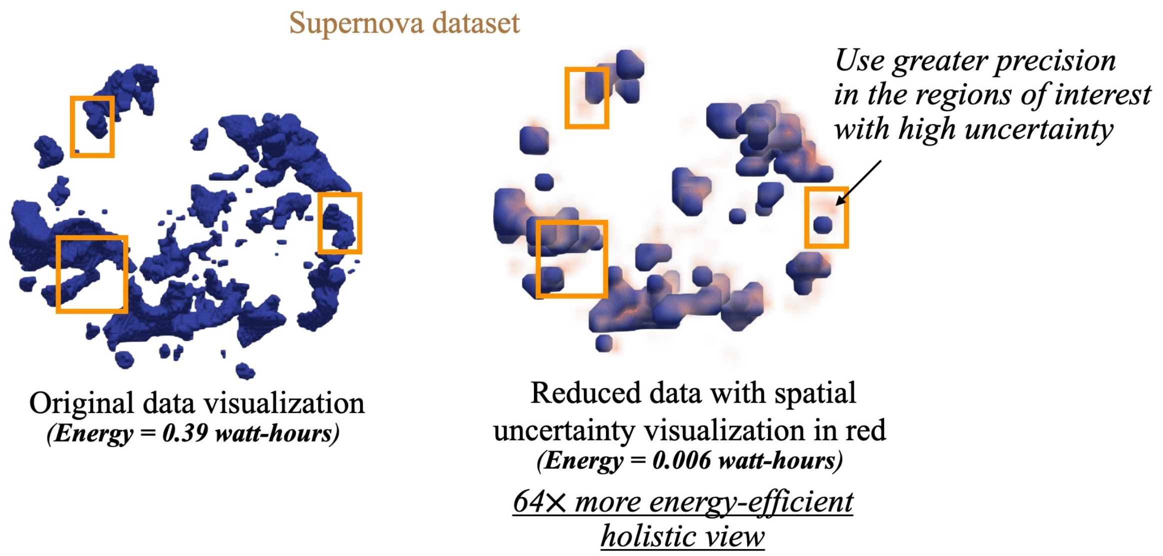
https://web.cvent.com/event/a3dd901a-699e-408c-8a84-81445e6ea64f/summary

Tushar M. Athawale, Oak Ridge National Laboratory

Uncertainty-Informed Approximate Computing for Energy-Efficient Visualization of Large Data

Opportunity and Potential Impact

- Visualization is key to gaining insights from large data but can be energy-inefficient.
- Main idea: Use uncertainty visualization as a mechanism to achieve maximal energy efficiency and accuracy.
- Impact: Uncertainty-informed visualization will help scientists to reliably analyze large data with minimal energy consumption.



State of the Art and Challenges

- Data approximations: ↑ energy efficiency, ↓ vis accuracy.
- Challenge: Without knowledge of uncertainty, a tradeoff between energy and precision cannot be understood.
- Understanding how data approximations (low precision, dimensionality reduction, interpolation) affect uncertainty and energy will need theoretical research, which is currently lacking.

Execution and Timeline

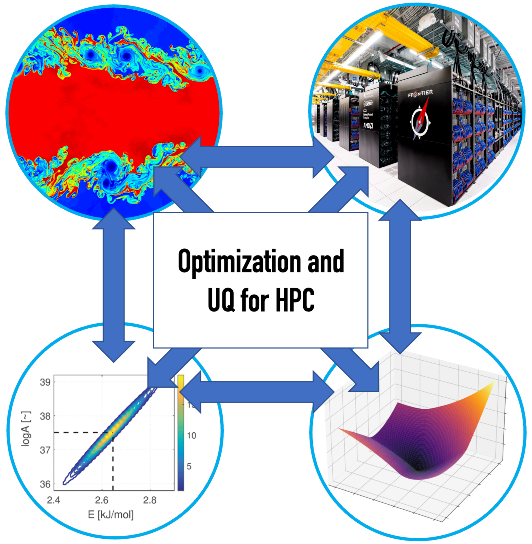
- Research thrusts: (1) How large data can be best approximated while capturing uncertainty (2) How uncertainty can be leveraged for energy efficiency.
- Barriers: Developing energy-efficient uncertainty vis algorithms will need rigorous statistical derivations and deriving novel visual mappings.
- Benchmarks: Original large data (e.g., see image above), alternative data approximations and uncertainty vis.

Tushar M. Athawale, Oak Ridge National Laboratory

Uncertainty-Informed Approximate Computing for Energy-Efficient Visualization of Large-Scale Data

Opportunity and Potential Impact

- What do you propose to do, minimal jargon
- Why now?
- What difference would a breakthrough make?
- How will we know we're on the right track, measure success?

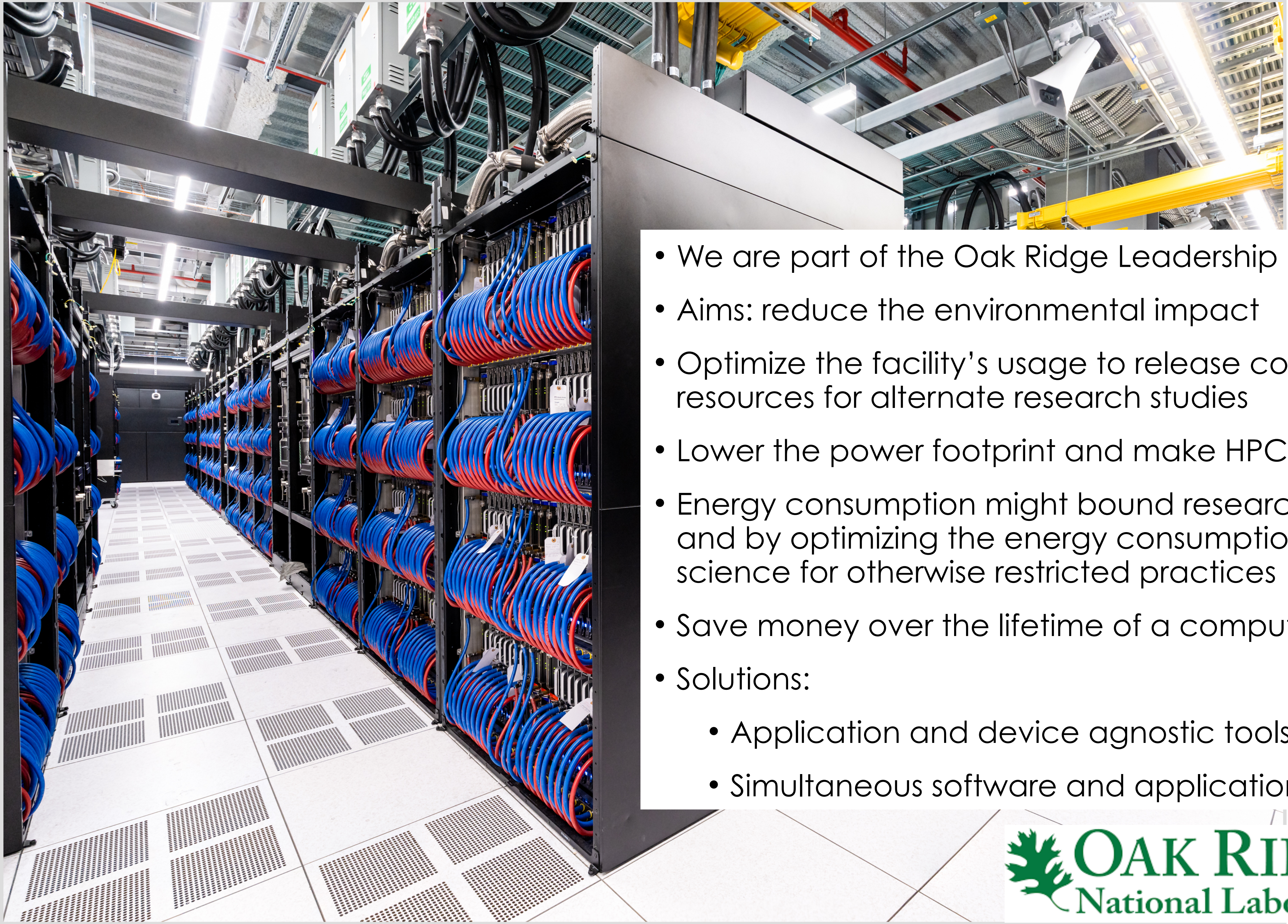


State of the Art and Challenges

- How is this done today, what are the shortcomings?
- Why is overcoming these challenges difficult?

Execution and Timeline

- What are some of the key steps along the way?
- How would you imagine this research and development unfolding over the next 5-10-15 years?
- What barriers to success can you anticipate?
- What resources (e.g., testbeds, data) would be necessary for success?

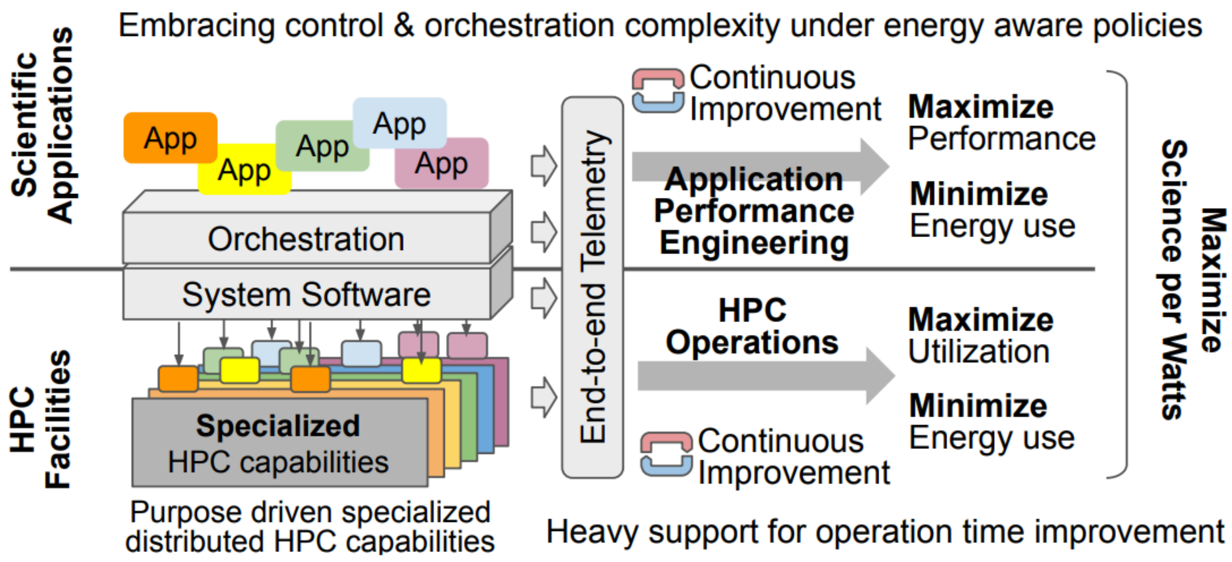


- We are part of the Oak Ridge Leadership Computing Facility
- Aims: reduce the environmental impact
- Optimize the facility's usage to release computational resources for alternate research studies
- Lower the power footprint and make HPC the choice
- Energy consumption might bound research projects and topics and by optimizing the energy consumption we might enable science for otherwise restricted practices
- Save money over the lifetime of a computing system
- Solutions:
  - Application and device agnostic tools
  - Simultaneous software and applications optimization for

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Towards Sustainable Post-Exascale Leadership Computing

- Strategy to optimize for EE the specialized OLCF hardware in targeted applications for **sustainable computing growth**
  - Hardware vendors should work hand in hand with the software developers to enhance the understanding for green practices
  - Software that targets utilizing the maximum of the resources provided for optimal science-per-watt results
  - Policies that ensure multi-tenancy for unused resources
  - Workflow tools and data management



Energy Constrained Post-exascale HPC Environment.

"Towards Sustainable Supercomputing", Shin W., White J. III, et al., SusSup24 at SC24

Data Sustainability and Workflows

- Data and energy efficiency:
  - Data centers
  - Data movement
  - Data storage
  - IRI initiatives
  - Implementation of data-driven operational analytics

Scientific applications and sustainability

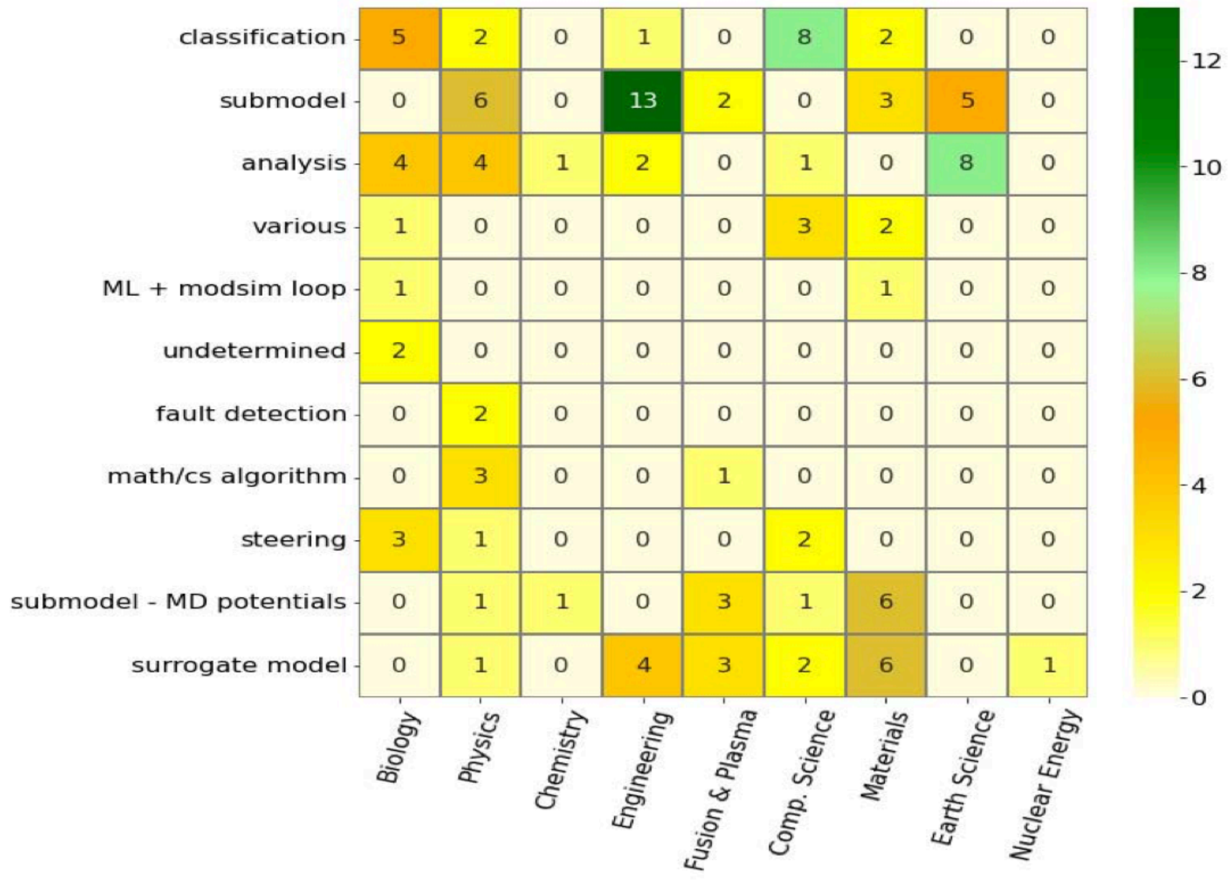
- Mixing computing technologies in a supercomputer to achieve lower cost and the best power per scientific output
- Aims: reduce the environmental impact
- Release computational resources for alternate research studies
- Lower the power footprint and make HPC the choice
- Energy consumption might bound research projects and topics and by optimizing the energy consumption we might enable science for otherwise restricted practices
- Save money over the lifetime of a computing system
- Solutions:
  - Application, platform, and device agnostic tools
  - Sustainable software
  - Best practices for policies discussions
- Optimize the Science per Energy Unit/Performance per Watt

Sustainable HPC growth

- Wider coverage solutions
  - Application and device agnostic power usage detection tools
  - Green software
  - Use GPU accelerators across applications (history of GPU usage)
  - Optimized operations data analytics
  - Operations: responsible utilization of resources
  - Complexity in the horizon including considering the trade-offs and effort to develop policies for accurate science with cost-efficient HPC

AI for science on a Leadership Supercomputer

- Increasing demands in user cases in AI/ML are a driving factor to changing the footing of energy consumption practices
- Not efficient: intensive lower precision usage and higher rates of data movement
- Catastrophology:
  - AI's energy consumption
    - Can contribute to climate change
    - Can strain electricity grids
    - Increase the demand for water for cooling data/HPC centers
-



AI motif vs. science domain, project counts.

Joubert W. et al, *URL:https://ieeexplore.ieee.org/document/9835678*

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Media on AI and Energy Footprint

- AI and data center growth equal power demand, American Nuclear Society, https://www.ans.org/news/article-5872/ai-and-data-center-growth-equal-power-demand/
- AI/data centers' global power surge and the Sustainability impact, The Goldman Sachs Group, Inc., https://www.goldmansachs.com/insights/articles/AI-poised-to-drive-160-increase-in-power-demand
- Powering Intelligence Analyzing Artificial Intelligence and Data Center Energy Consumption (EPRI), https://www.wpr.org/wp-content/uploads/2024/06/3002028905_Powering-Intelligence_-Analyzing-Artificial-Intelligence-and-Data-Center-Energy-Consumption.pdf
- Powering the AI Revolution, Morgan Stanley, https://www.morganstanley.com/ideas/ai-energy-demand-infrastructure
- Carbon Footprint of Data Centers & Data Storage Per Country (Calculator), 8 Billion Trees, https://8billiontrees.com/carbon-offsets-credits/carbon-ecological-footprint-calculators/carbon-footprint-of-data-centers/#:~:text=Data%20centers%20account%20for%202.5,that%20fuel%20the%20global%20economy
- AI's Growing Carbon Footprint, Columbia Climate School, https://news.climate.columbia.edu/2023/06/09/ais-growing-carbon-footprint/
- The Decoder, GPT-4 has more than a trillion parameters - Report, https://the-decoder.com/gpt-4-has-a-trillion-parameters/#:~:text=Further%20details%20on%20GPT-4's,Mixture%20of%20Experts%20(MoE). AI's Growing Carbon Footprint, Columbia Climate School, https://news.climate.columbia.edu/2023/06/09/ais-growing-carbon-footprint/

AI for science on a Leadership Supercomputer

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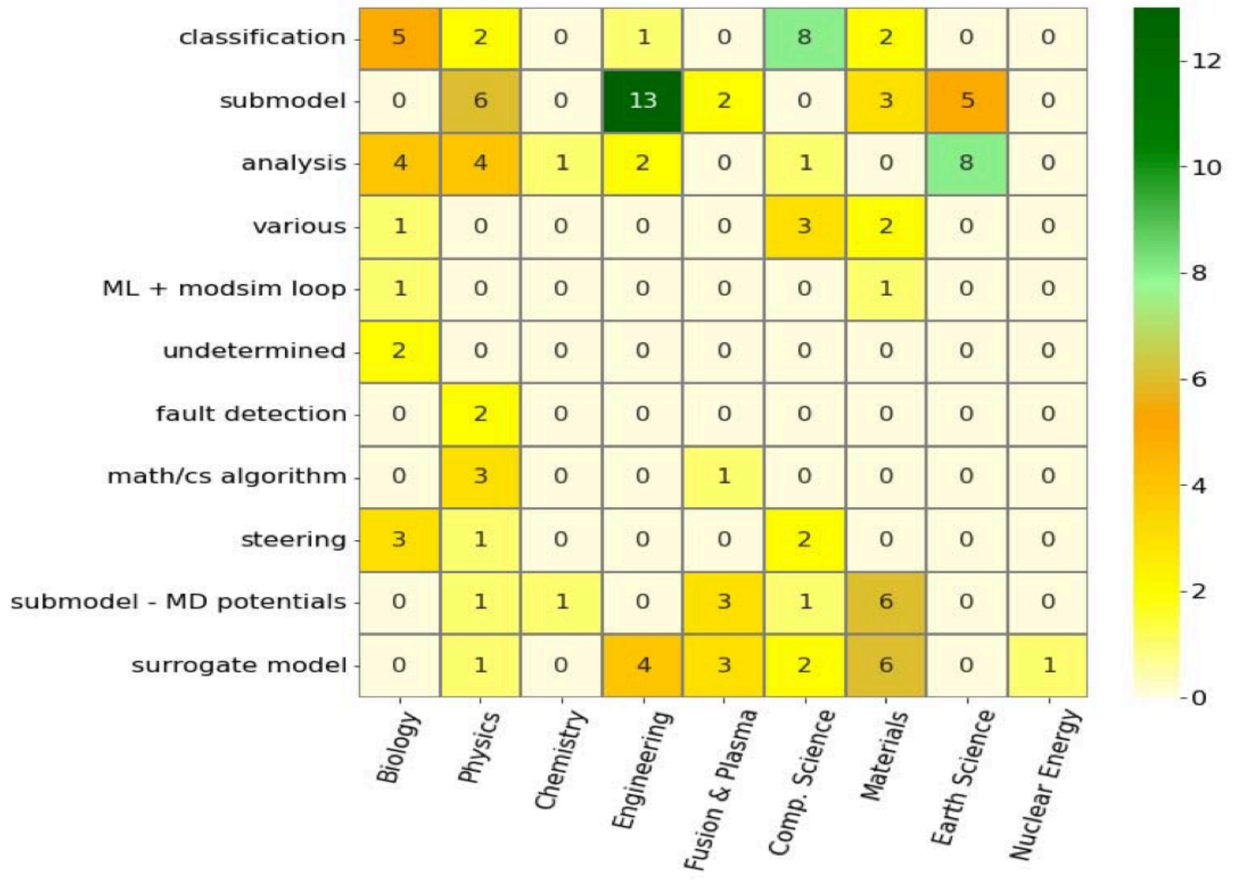
- Not efficient: intensive lower precision usage and higher rates of data movement
- Catastrophology:
  - AI's energy consumption
    - Can contribute to climate change
    - Can strain electricity grids
    - Increase the demand for water for cooling data/ HPC centers
- Strategies to mitigate those effects:
  - Retraining on better data
  - Model pruning/optimization to remove the redundant
  - Source code enhancements
  - Deployment modification to optimize the results
  - Regularize to treat undercutting and overfitting



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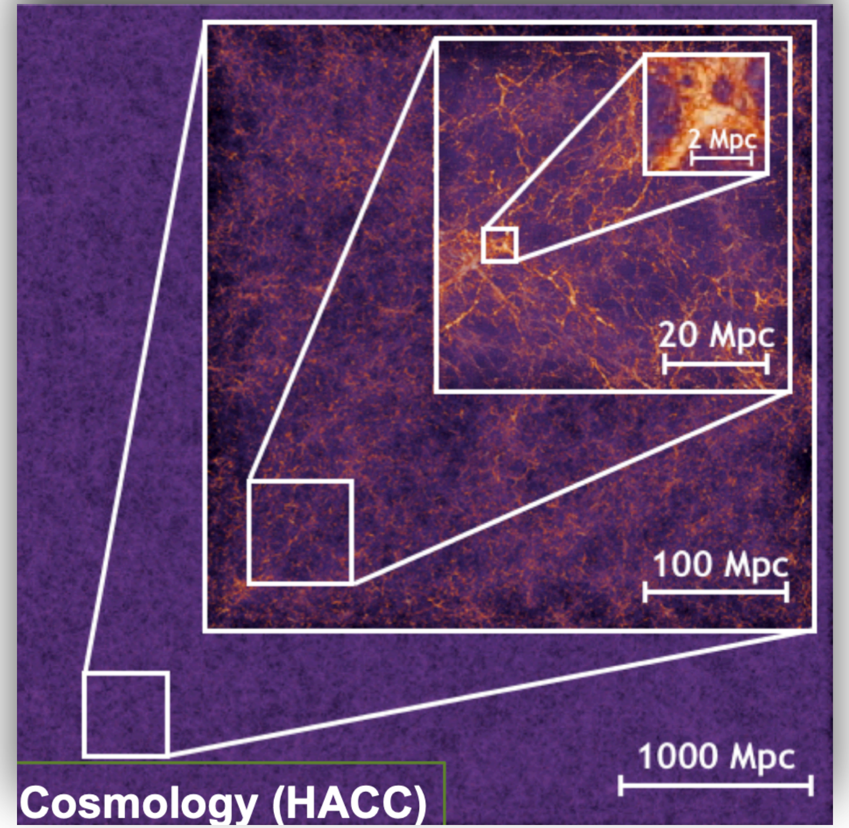
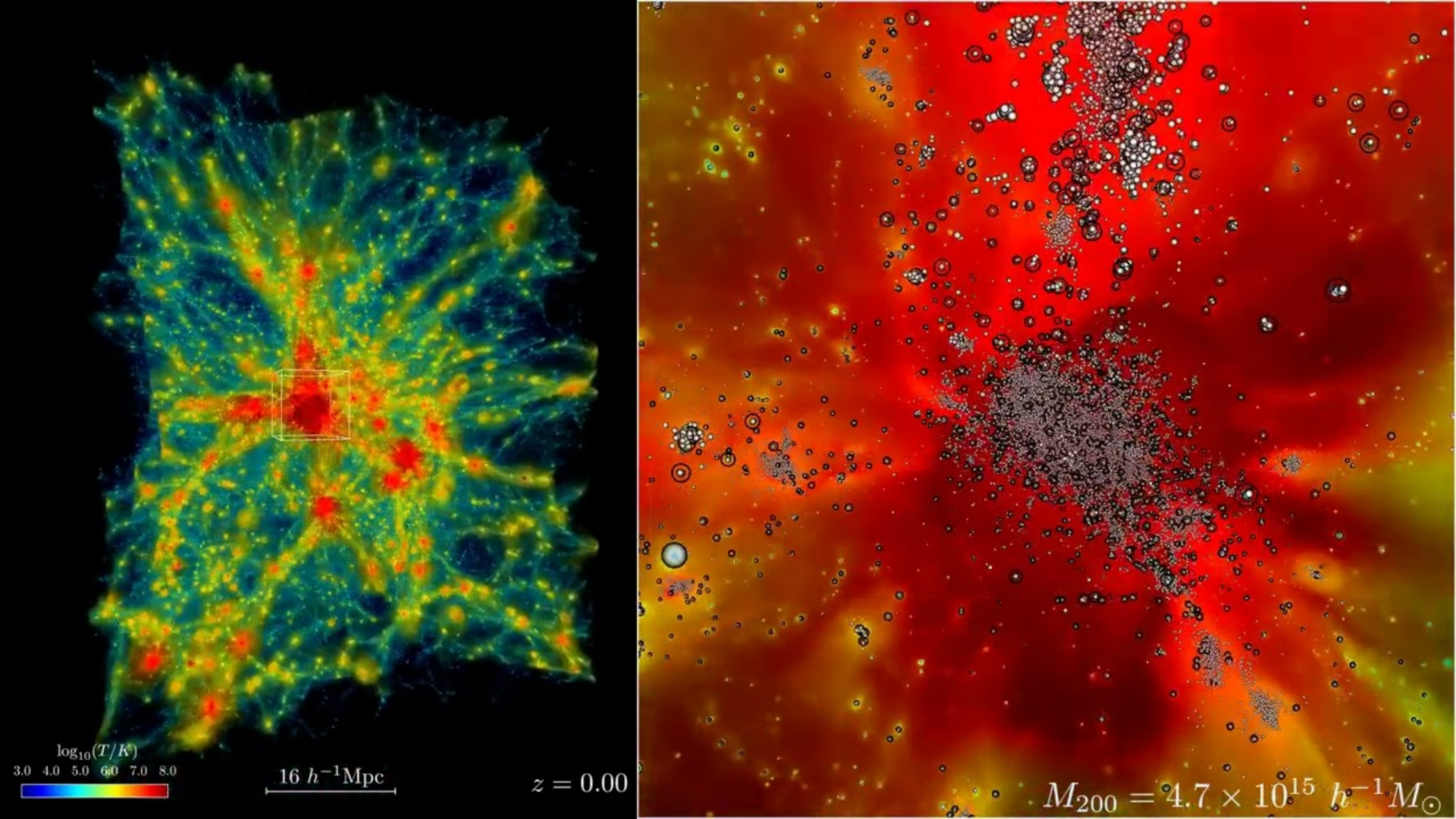
HACC: Computing the Sky at Extreme Scales

Or Fitting the Universe in a simulation and running it on a supercomputer

- Enable the extraction of fundamental physics from upcoming cosmological surveys
- Explore dark matter/dark energy
- Understand and characterize systematics
- Scientific Challenge Problem
  - HACC **gravity-only simulation** as foundation for most detailed synthetic sky maps ever made
  - HACC **hydro simulation** to understand the effects of baryons on cosmological probes
  - Relevant scales: groups and clusters
  - Relevant physics: AGN, SNe



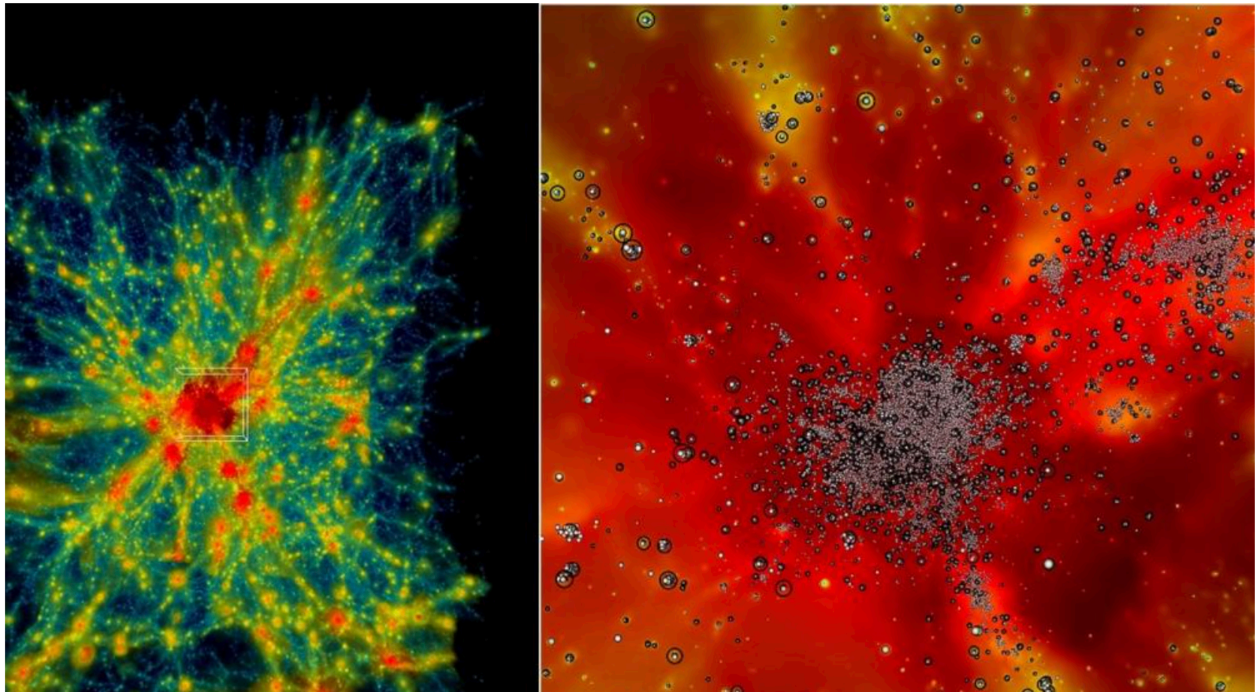
Zoom-in visualization of the density field in a 1.07 trillion particle simulation with HACC (arXiv:1410.2805)



$\log_{10}(T/K)$
3.0 4.0 5.0 6.0 7.0 8.0
16 h^{-1}Mpc
$z = 0.00$
$M_{200} = 4.7 \times 10^{15}\ h^{-1} M_\odot$

“The universe just got a whole lot bigger…”

Record-breaking run on Frontier sets new bar for simulating the universe in the exascale era



RESEARCHERS

Bronson E Messer II

Organizations

- Computing and Computational Sciences Directorate
- User Facilities
- Oak Ridge Leadership Computing Facility

https://www.ornl.gov/news/record-breaking-run-frontier-sets-new-bar-simulating-universe-exascale-era

HACC- Hardware/Hybrid Accelerated Cosmology Code

HACC was developed to performantly run simulations on all modern supercomputing platforms, scaling to millions of cores and exploiting heterogeneous hardware such as graphics processing units (GPUs)

- HACC Code Characteristics
  - HACC is C++ & MPI and can adapt to OpenCL, CUDA, Cell SDK, HiP etc
  - Algorithm Co-Design
    Multiple algorithm options, stresses accuracy, low memory overhead, no external libraries in simulation path
- Short range force calculation
  - HACC uses a hybrid algorithm in its gravity solver:
    short-range computation consumes most of the simulation time—> tuned to the system architecture

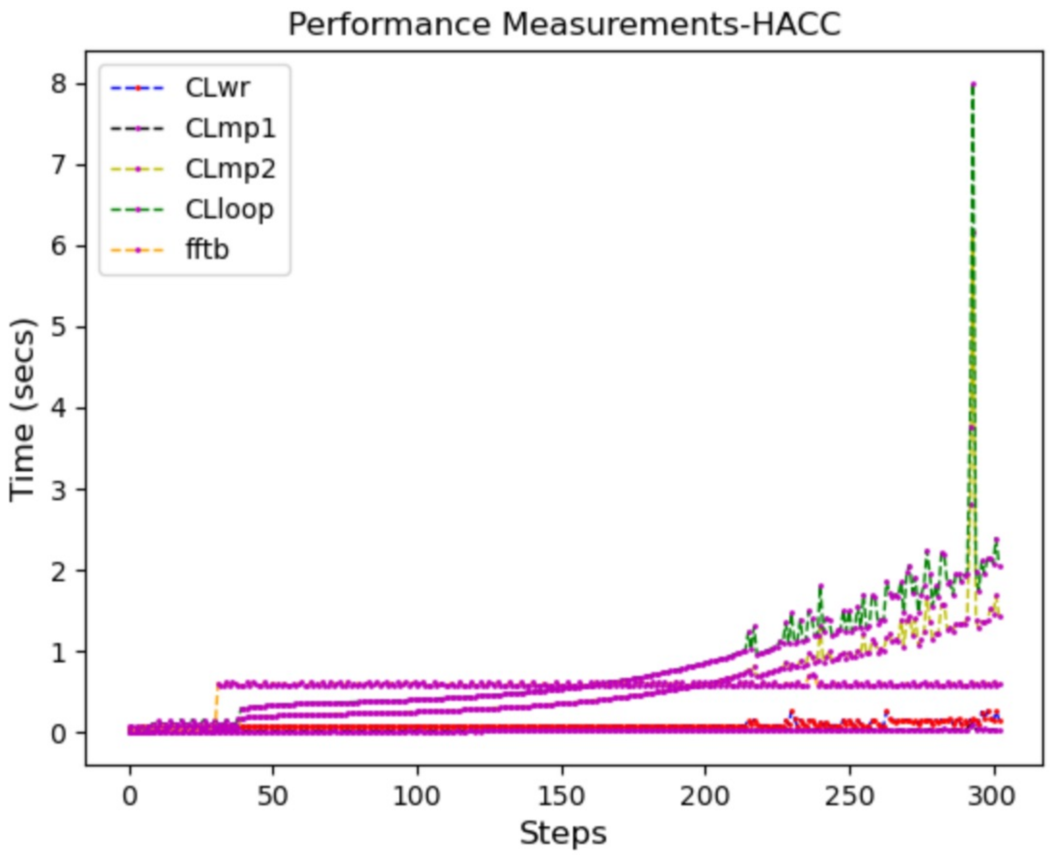
$$\mathrm{FOM} = \sqrt{\left(\frac{n_p^3}{t}\right)_{\mathrm{grav}} \left(\frac{2n_p^3}{t}\right)_{\mathrm{hydro}}}$$

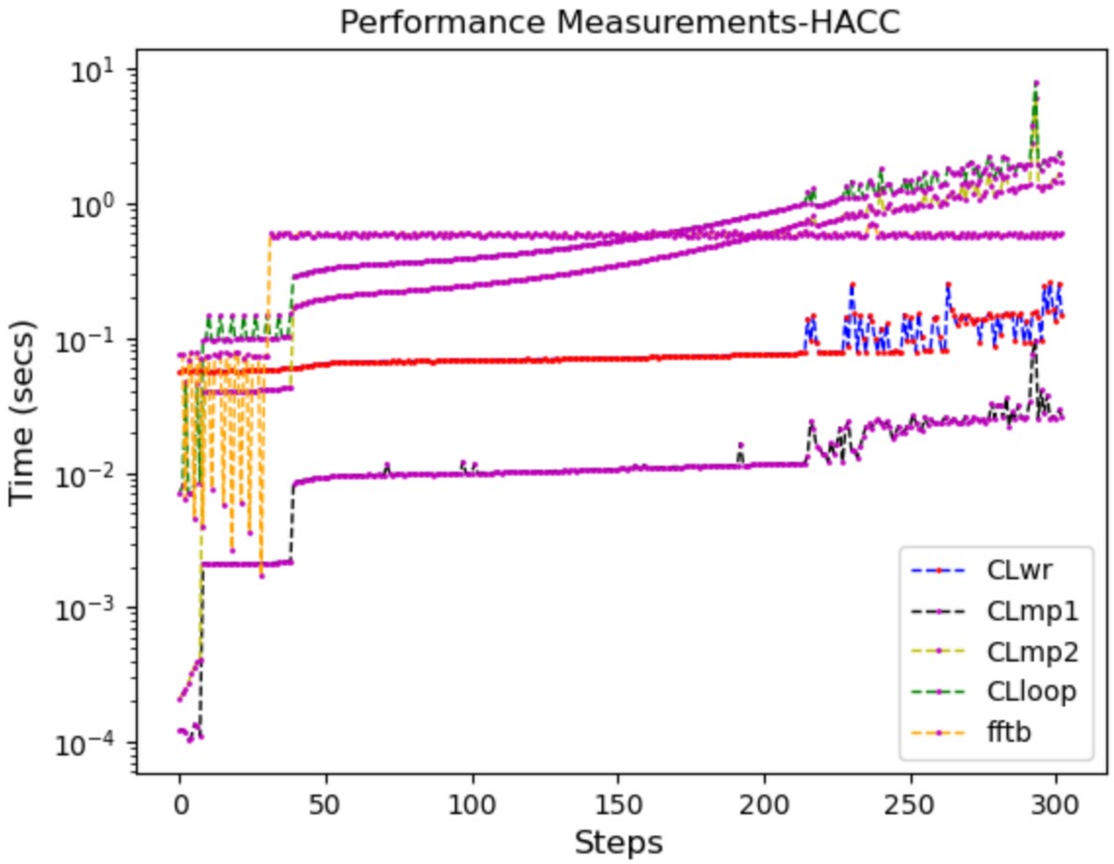
Machine	# nodes	FOM	$\mathrm{FOM}^{\mathrm{ext}}$
Summit	4096	64.22	72.25
Frontier	4096	122.47	140.65
Frontier	6144	181.64	208.60
Frontier	8192	233.68	268.36
Frontier	8192	236.54	271.65

https://dl.acm.org/doi/10.1145/3581784.3607065

https://doi.org/10.1145/3581784.3607089

Without a profiling tool- 1000 nodes, gravity-only





sacct -j <jobid> -D --format=User,JobID,JobName,ConsumedEnergyRaw

- Used to view accounting data for jobs and job steps in the accounting log (in queue or recently completed).

User JobID	JobName	Consumed Energy Raw
2504271	hacc_grav	4094824029
2504271.bat+	batch	3973157
2504271.ext+	extern	4094824029
2504271.0	hacc_p3m	3753861065

The **sacct** command will show running job accounting data stored in the job accounting log file or Slurm database in a variety of forms

Trey White

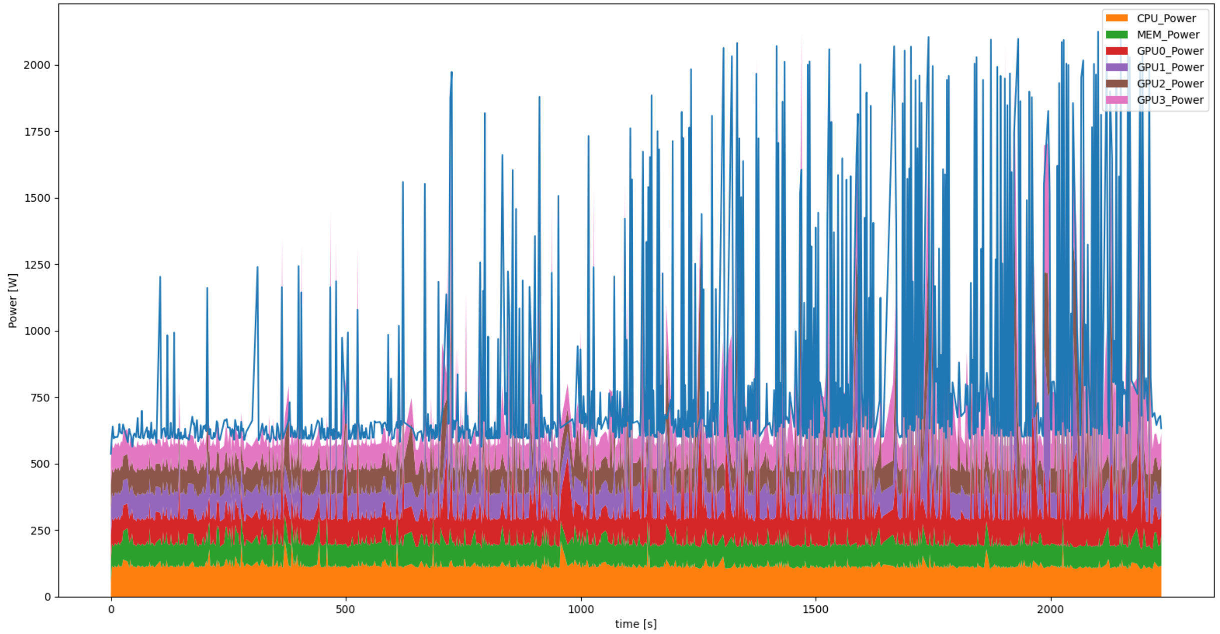
1 node- (256x256) NP

User	JobID	JobName	ConsumedEnergyRaw
antigoni	214489	cosmo_grav	1413315
	214489.batch	batch	1413084
	214489.exte+	extern	1413315
	214489.0	hacc_p3m	62

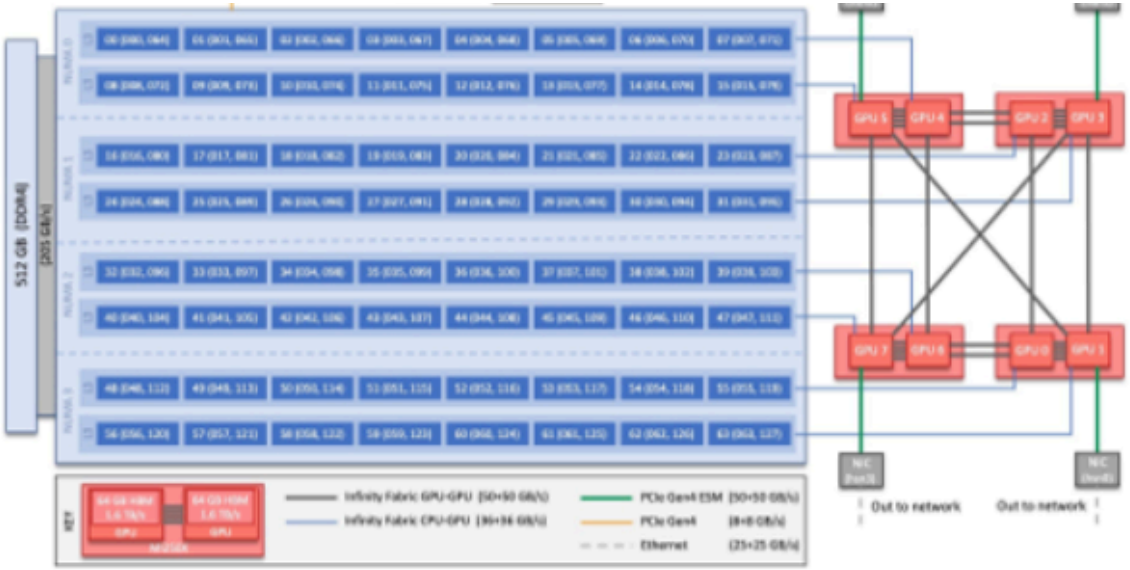
JobID	JobName	ConsumedEnergyRaw	Start	End	State
214489	cosmo_grav	1413315	2024-10-03T14:12:12	2024-10-03T14:36:58	COMPLETED
214489.batch	batch	1413084	2024-10-03T14:12:12	2024-10-03T14:36:58	COMPLETED
214489.exte+	extern	1413315	2024-10-03T14:12:12	2024-10-03T14:36:58	COMPLETED
214489.0	hacc_p3m	62	2024-10-03T14:12:16	2024-10-03T14:36:58	COMPLETED

HACC with CrayMP

Dr. Matthias Maiterth



OLCF Frontier cabinets deployed at ORNL



Frontier node showing Non-Uniform Memory Architecture characteristics and complex linkages between CPU, GPU, memory, and network interfaces

Mixed Precision support in HPC applications: What about reliability?

	Benchmarking	Molecular Dynamics and Biology	Quantum Chemistry	Lattice Quantum Chromodynamics	Computational Fluid Dynamics	Cosmology and Plasma Physics	Geology	Weather Modeling
SP Support		MiniMD [71]		BQCD [83] MILC [13] CHROMA [40]	OpenFOAM [21] MiniFE [11]	LareXD [5]	SPECFEM3DG [92] SeisSol [20] EFISPEC3D [94] YASK [111] CPML [17]	WRF [99] MiniWeather [22]
MP Support	HPL-AI [62] MixPB [91]	LAMMPS [104] GROMACS [2] HMMER [42] AMBER [26]	QMCPack [58]	GRID [19] HotQCD [4] OpenQCD [24]		GADGET [101] HACC [48]		SILAM [100] CAMx [103] IFS [107] AROME [98] ICON [112] UM [79]
DP Support Only	HPL [39] HPCG [38] HPCC [75] NPB [10] STREAM [16]	NAMD [93]	QE [45] CP2K [63] NWChem [106] VASP [49] Siesta [6] Qbox [47] LSMS [109] MiniDFT [8]		Nek5000 [87] Lulesh [56] Laghos [60] Remhos [60] Cloverleaf [76] PENNANT [41]	iPIC3D [77] FLASH [44] UMT [52] SNAP [113] Kripke [66] Quicksilver [95]	SW4 [90]	CMAQ [103] NEMO [80]

- Assorted scientific domain test cases with respect to their nominal recision usage on HPC
  - Use of floating-point mixed precision is widespread across all domains of HPC
  - Weather Modeling is at the forefront of mixed precision production use in HPC
  - Use of single and mixed precision leads to a higher Silent Data Error (SDE) rate
  - The severity of observed SDEs is much higher under single and mixed precision

Netti A. et al, https://doi.org/10.1016/j.jpdc.2023.104746

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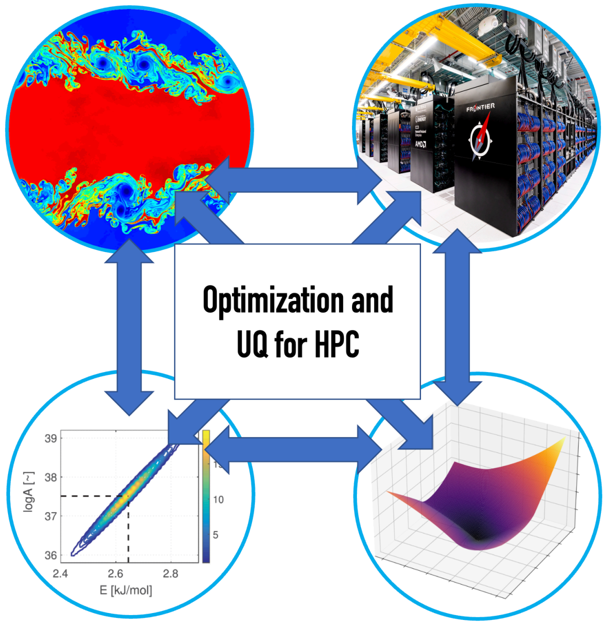
Uncertainty Quantification in science and engineering prediction

<u>Understanding the origins of and assessing the magnitudes of the errors which accompany computer simulations</u>

- Uncertainty is a fundamental quantum physical concept
- Arises in our macroscopic observations of the physical world
- The uncertainty quantification community develops methods to accelerate both forward propagation of uncertainty, and inverse UQ (i.e. calibrating uncertainties using data)
  - challenging when models are expensive
  - Traditional “guess-and-check” methods- less performant and more expensive
- Exascale: expected to see more of these existing uncertainty propagation methodologies embedded within or wrapped around deterministic simulation codes
  - Sampling-based methods repeatedly call a deterministic simulation code for different values of the model inputs
  - Independent instantiations of this method makes it a good fit for parallel programming paradigms and deployment to compute nodes in different HPC systems

Conclusions

- Supercomputing is important:
  - hard problems to solve
  - scientific discoveries in complex system like materials, astrophysics, biology
  - theoretical domains, are a many-component system-scale simulations
  - large scale inverse problems, like optimization
  - data-intensive computing



- Uncertainty Quantification
  - Strategies for overcoming supercomputing bottlenecks: impact of queue policies and restrictions on scientific workflows, limitations with I/O and methods for I/O coupling, mixed-language and mixed-precision computing, and general memory/compute limitations

https://epsouqhpc.ornl.gov/

Come and Compute with Us at OLCF!!!

- Did you know that ~60% of our cycles are available via the DOE INCITE program?
  - Anyone can apply, worldwide!
  - Successive applicants get liaisons like me to help them reach their science goals.
  - The deadline for INCITE proposals for 2023 has passed... but there is always next year
  - visit: https://www.doeleadershipcomputing.org/
- Up to ~25% of our cycles go to the ASCR Leadership Computing Challenge (ALCC):
  - visit: https://science.osti.gov/ascr/Facilities/Accessing-ASCR-Facilities/ALCC

OLCF Frontier Cabinets deployed at ORNL

If you really need these computational resources & computational power there is no substitute

Contact me: georgiadoua@ornl.gov

Resources- Literature- Media

- https://conferences.computer.org/sc-wpub/pdfs/SC-W2024-6oZmigAQfgJ1GhPL0yE3pS/555400b496/555400b496.pdf
- https://www.bu.edu/peaclab/files/2024/10/Analysis-of-Power-Consumption-and-GPU-Power-Capping-for-MILC_CameraReady.pdf
- https://web.cvent.com/event/a3dd901a-699e-408c-8a84-81445e6ea64f/websitePage:4f5780f1-9811-4588-8a98-fb418e1b1636
- https://rocm.github.io/omnitrace/
- https://rocm.docs.amd.com/projects/rocm_smi_lib/en/latest/index.html
- https://confluence.ccs.ornl.gov/download/attachments/389972596/ADAC13_NVIDIA_wells_Presentation[54].pptx?version=1&modificationDate=1719936780387&api=v2
- https://www.science.org/content/article/climate-modelers-grapple-their-own-carbon-emissions
- https://github.com/eas4dc/EAR
- https://top500.org/lists/green500/
- https://cpe.ext.hpe.com/docs/latest/performance-tools/man5/cray_pm.html
- https://rmets.onlinelibrary.wiley.com/doi/full/10.1002/qj.4181
- https://slurm.schedmd.com/power_save.html
- https://arxiv.org/abs/2412.19322
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Discussion