From Petaflops to Energy Solutions

A Cross-Sectoral Analysis of High-Performance Computing in Energy Research

Introduction

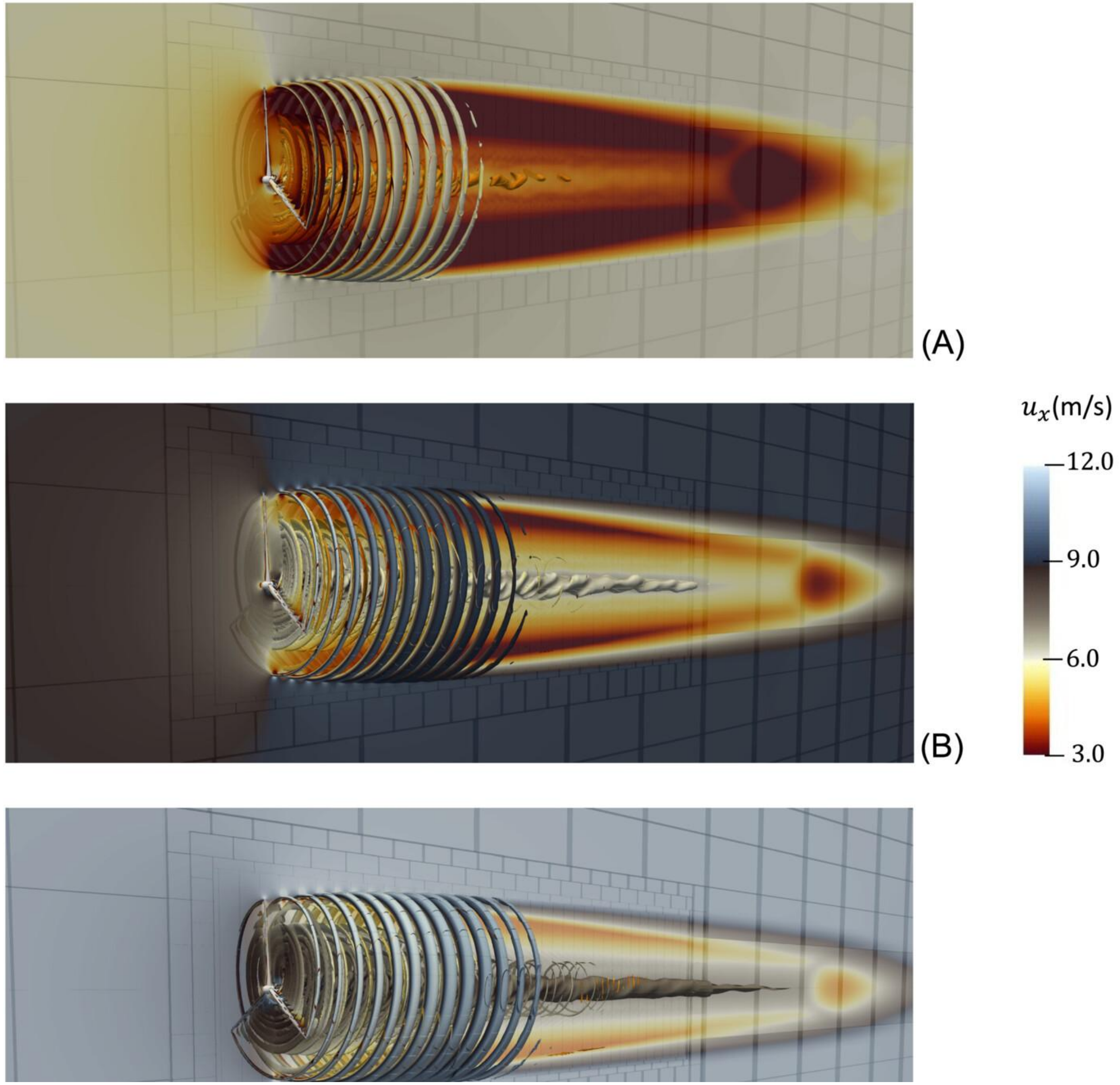
- Energy research is one of the most pressing topics of the 21st century
- HPC has become central to energy research efforts
- Computational needs in energy research continue to grow
- The US Department of Energy (DOE) oversees most supercomputers in the US

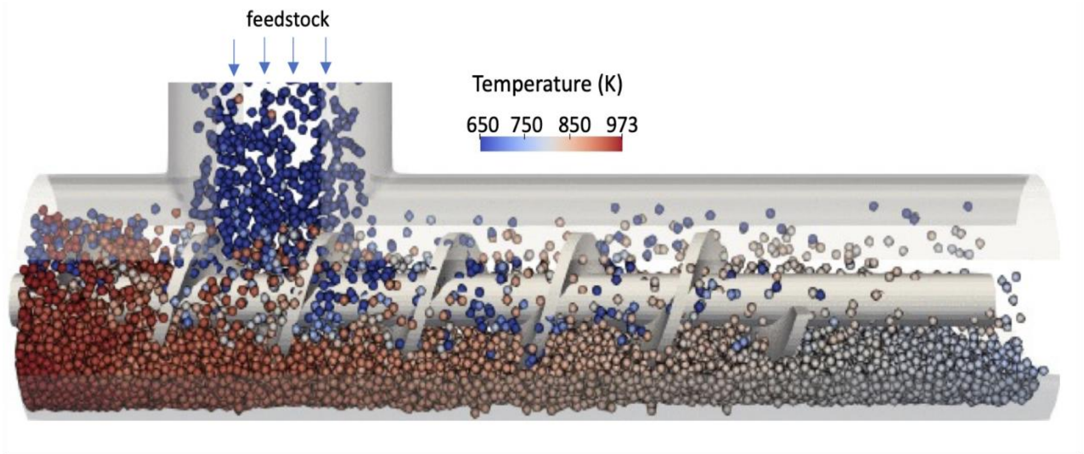
Historical Connection: HPC and Energy

- Manhattan Project (1943): First use of computing in energy research
- IBM punch-card machines for nuclear calculations
- Post-war: Computers became essential for hydrogen bomb design
- MANIAC computer (1952): Los Alamos developed world's largest HPC center
- This established the tight relationship between HPC and DOE

Renewable Energy: Wind

- ExaWind framework: Physics-based modeling for wind flow simulation
- Collaboration between NREL, Oak Ridge, UT Austin, Sandia
- Leverages MPI for parallelism and GPU acceleration
- Used to study blade erosion, pitch-control, and vibrations



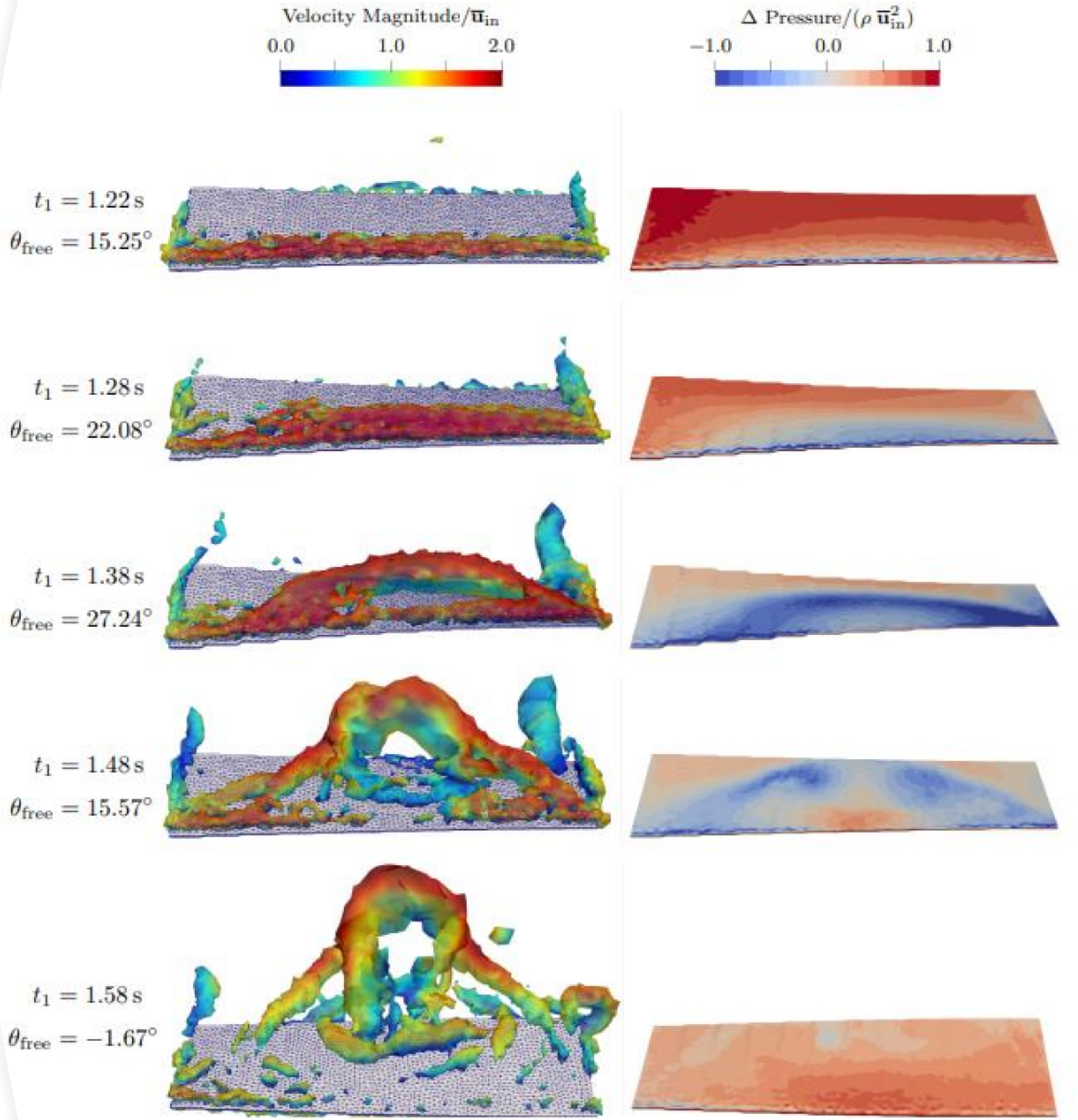


Renewable Energy: Biofuels

•BDEM (Biomass Discrete Element Method)
•Simulates granular flow of biomass material
•Models transportation of renewable carbon sources
•Helps reduce maintenance costs by addressing hopper jamming issues

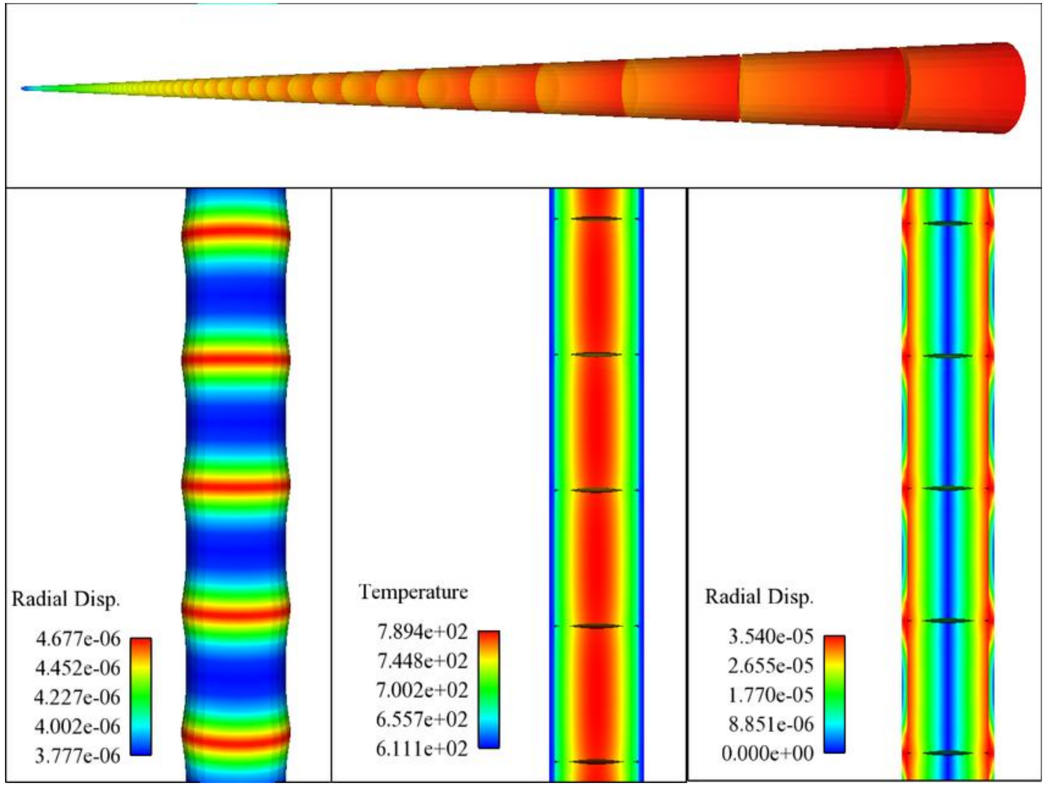
Renewable Energy: Solar Power

- PVade: Fluid-structure interaction model for solar arrays
- Studies wind effects on photovoltaic panels
- Simulates torsional galloping that damages solar panels
- Machine learning techniques used to accelerate simulations



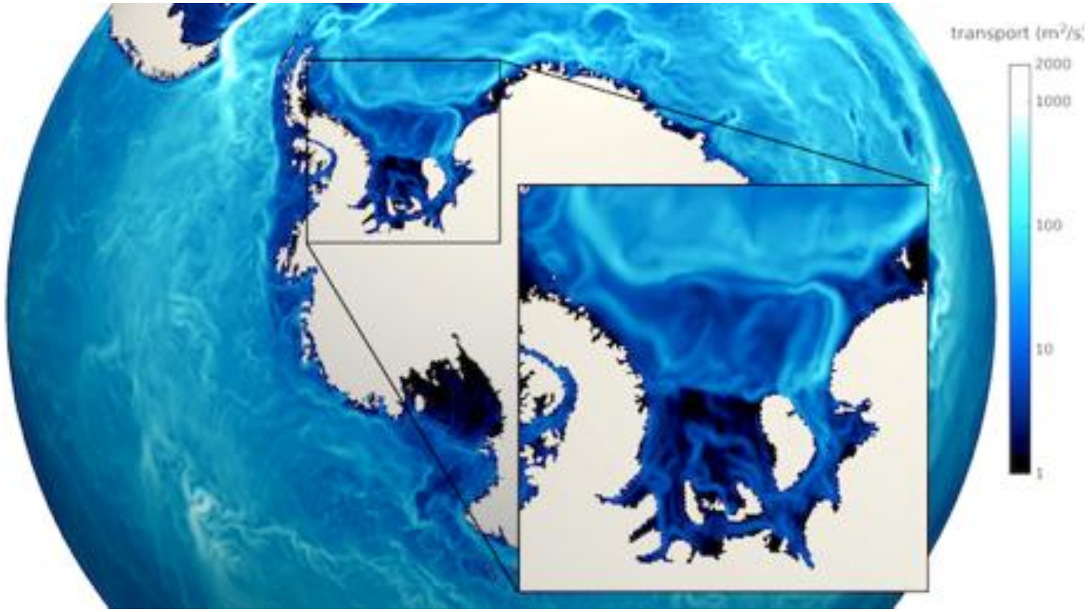
Renewable Energy: Nuclear

- Nuclear provides ~20% of US energy mix
- MOOSE (Multiphysics Object-Oriented Simulation Environment)
- Developed by Idaho National Laboratory
- Allows simulation of fuel rods with temperature profiles and displacement
- Enables advances without dangerous physical experiments



Environment: Climate Modeling

- Energy Exascale Earth System Model (E3SM)
- Achieves simulation resolutions 30x finer than existing models
- Improves accuracy of climate phenomena modeling
- Studies water cycle, biogeochemical cycles, and cryosphere-ocean interactions

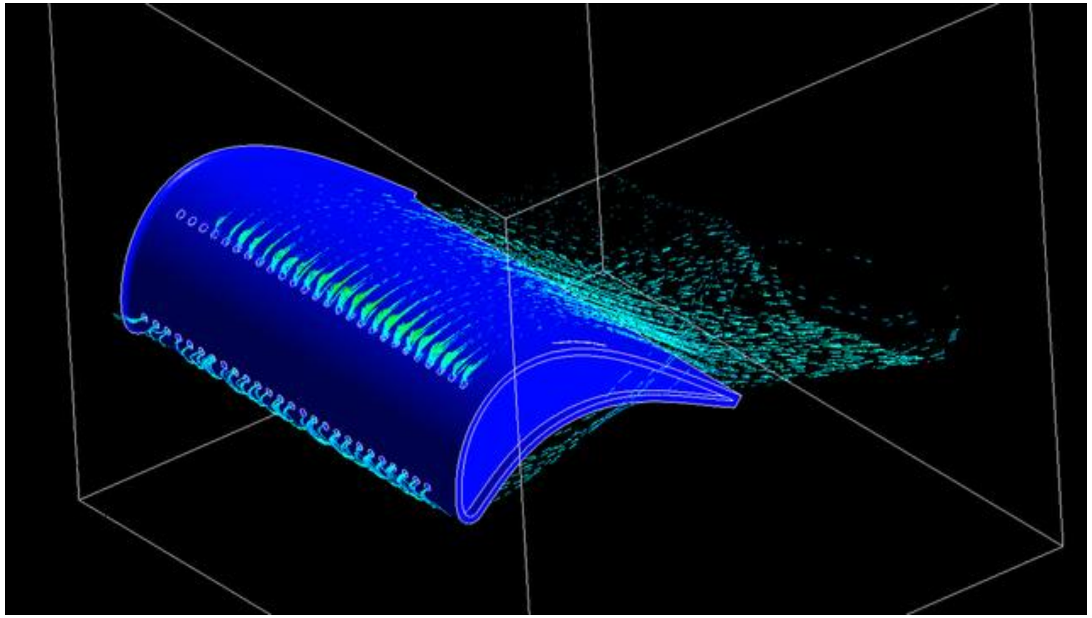


Environment: De-carbonization

- Iron and steel-making account for 7-9% of global greenhouse emissions
- HPC projects aim to introduce electrification and clean energy
- Example: Development of 100% hydrogen-based furnaces
- Simulation needed as measurements in high-temperature environments are difficult

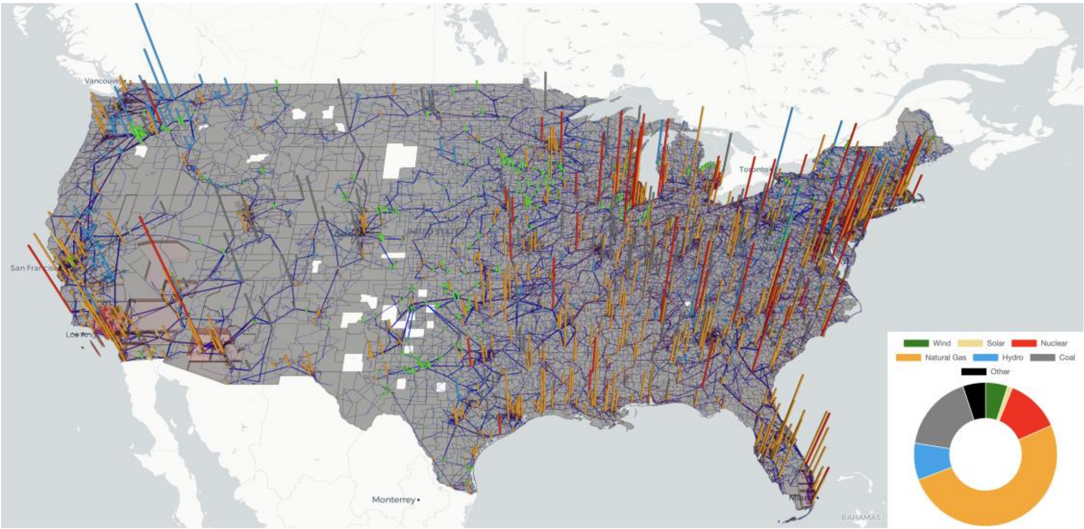
Energy Efficiency: Engine Design

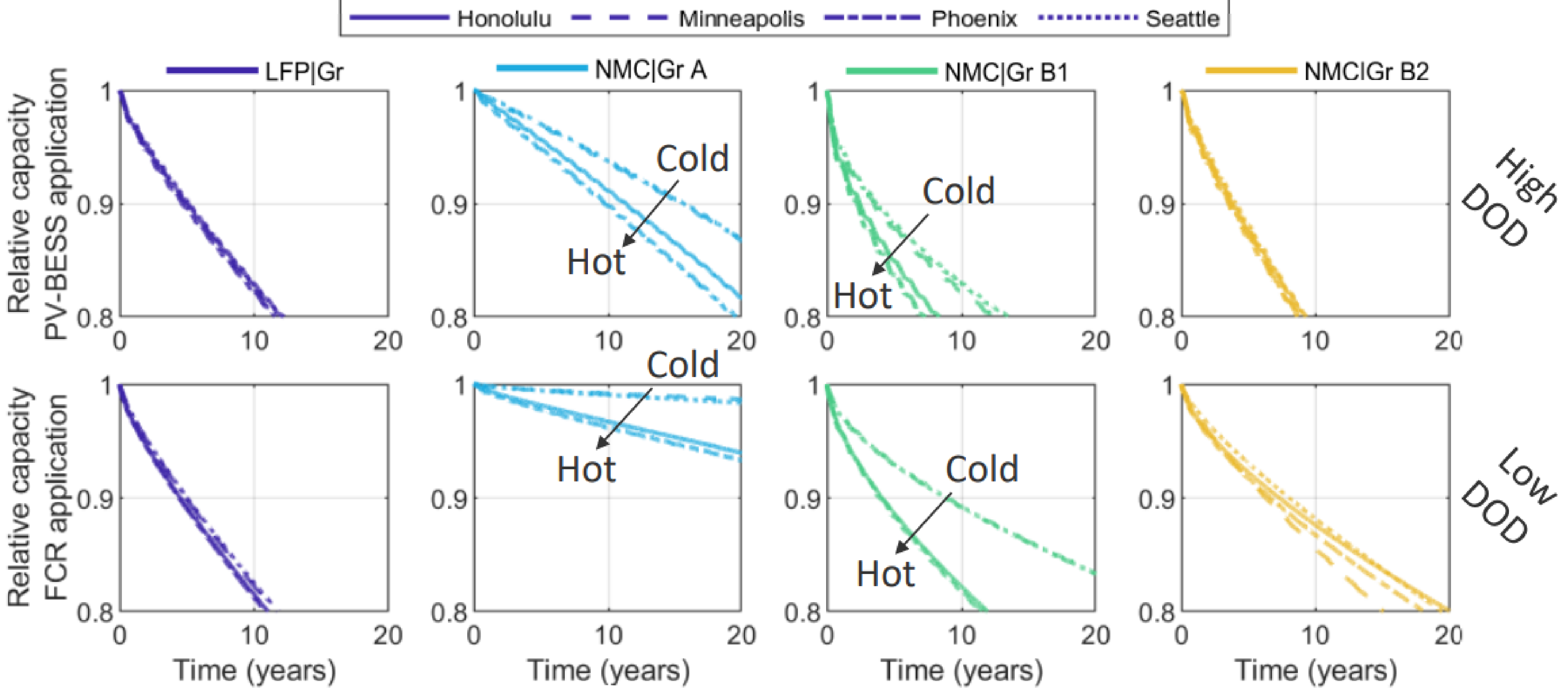
- Collaboration between Raytheon and Argonne
- Optimizes cooling of internal engine components
- 10% reduction in cooling air can lead to 1% reduction in fuel consumption
- Uses computational fluid dynamics with machine learning acceleration



Energy Efficiency: Power Grid

- National grid is backbone of energy infrastructure
- ExaSGD framework for power grid simulation
- Models how renewables impact grid reliability
- Helps balance energy loads and develop resilient systems





Energy Efficiency: Battery Technology

- •BLAST: Battery Lifetime Analysis and Simulation Tool suite
- •Models degradation of lithium-ion batteries
- •Uses publicly available data from manufacturers
- •Predicts performance under various weather conditions

Future Implications

•Energy security critical for economic stability
•Climate change mitigation requires efficient energy solutions
•Integration of renewables introduces grid reliability challenges
•Storage capacity key to enabling green transition
•National security concerns drive energy research

Conclusion

- HPC is imperative for modern energy research
- Advances benefit from both weak and strong scaling
- Energy research can shape future generations by:
    - Reducing cost of living
    - Fighting climate change
- Funding for HPC in energy applications is crucial

References

- [1] URL: https://github.com/Exawind.
- [2] Aly Mousaad Aly and John Clarke. “Wind Design of Solar Panels for Re-silient and Green Communities: CFD with Machine Learning”. In: Sustain-able Cities and Society Accepted. (Mar. 2023). DOI: 10.1016/j.scs.2023.104529.
- [3] P. M. Caldwell et al. “Convection–Permitting Simulations With the E3SMGlobal Atmosphere Model”. In: Journal of Advances in Modeling Earth Sys-tems 13.11 (Nov. 2021). ISSN: ISSN 1942-2466. DOI: 10.1029/2021ms002544.URL: https://www.osti.gov/biblio/1833211.
- [4] Nicholas Deak et al. “A high-performance discrete-element framework forsimulating flow and jamming of moisture bearing biomass feedstocks”. In:Powder Technology (2024), p. 120548. DOI: 10.1016/j.powtec.2024.120548. URL: https://doi.org/10.1016/j.powtec.2024.120548.
- [5] Nicholas Deak et al. “A high-performance discrete-element framework forsimulating flow and jamming of moisture bearing biomass feedstocks”. In:Powder Technology 452 (2025), p. 120548. ISSN: 0032-5910. DOI: https:/ / doi . org / 10 . 1016 / j . powtec . 2024 . 120548. URL: https : / / www .sciencedirect.com/science/article/pii/S0032591024011926.
- [6] DoE. Computers in the Manhattan Project. URL: https://www.osti.gov/opennet/manhattan-project-history/Science/ParticleAccelerators/computer.html.
- [7] E3SM-Project. The Multiphysics Object-Oriented Simulation Environment(MOOSE). URL: EnergyExascaleEarthSystemModel(E3SM).
- [8] ECP. The Exascale Computing Project (ECP). URL: https://www.exascaleproject.org/.

References

- [9] Derek Gaston et al. “Parallel Algorithms and Software for Nuclear, Energy,and Environmental Applications. Part II: Multiphysics Software”. In: Com-munications in Computational Physics 12 (Sept. 2012). DOI: 10.4208/cicp.091010.140711s.
- [10] Derek Gaston et al. “Parallel multiphysics algorithms and software for com-putational nuclear engineering”. In: Journal of Physics Conference Series180 (Aug. 2009), p. 012012. DOI: 10.1088/1742-6596/180/1/012012.
- [11] hpc4energyinnovation. Microwave-assisted Ceramic Processing. URL: https:// / hpc4energyinnovation . llnl . gov / success - stories / microwave -assisted-ceramic-processing.16
- [12] Idaho National Lab. The Multiphysics Object-Oriented Simulation Environ-ment (MOOSE). URL: https://github.com/idaholab/moose.
- [13] MREL. Battery Lifetime Analysis and Simulation Toolsuite (BLAST). URL:https://github.com/NREL/BLAST-Lite.
- [14] Nrel. NREL/pvade: PVade is a fluid-structure interaction solver for studyingwind loading and aerodynamic stability in solar-tracking PV arrays. URL:https://github.com/NREL/PVade.
- [15] Vimal Ramanuj et al. Modeling the Effects of Microwave Heating on Den-sification in Chemical Vapor Infiltration. Tech. rep. Oak Ridge NationalLaboratory (ORNL), Oak Ridge, TN (United States), Apr. 2023. DOI: 10.2172/1971031. URL: https://www.osti.gov/biblio/1971031.
- [16] Ashesh Sharma et al. “ExaWind: Open-source CFD for hybrid-RANS/LESgeometry-resolved wind turbine simulations in atmospheric flows”. In: WindEnergy 27.3 (2024), pp. 225–257. DOI: https://doi.org/10.1002/we.2886. eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/we.2886. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/we.2886.
- [17] Ethan Young et al. “A fluid-structure interaction solver for investigatingtorsional galloping in solar-tracking photovoltaic panel arrays”. In: Journalof Renewable and Sustainable Energy 12.6 (Nov. 2020), p. 063503. ISSN:1941-7012. DOI: 10.1063/5.0023757. eprint: https://pubs.aip.org/aip/jrse/article-pdf/doi/10.1063/5.0023757/15777696/063503_1_online.pdf. URL: https://doi.org/10.1063/5.0023757.