Advanced Scientific Computing Research (ASCR)

Scientific Discovery through Advanced Computing (SciDAC)

Hal Finkel and the ASCR SciDAC Team

https://science.osti.gov/ascr/officehours

Office of Science (SC) Statement of Commitment & other Guidance

- **SC Statement of Commitment** – SC is fully and unconditionally committed to fostering safe, diverse, equitable, inclusive, and accessible work, research, and funding environments that value mutual respect and personal integrity. https://science.osti.gov/SW-DEI/SC-Statement-of-Commitment
- **Expectations for Professional Behaviors** –SC's expectations of all participants to positively contribute to a professional, inclusive meeting that fosters a safe and welcoming environment for conducting scientific business, as well as outlines behaviors that are unacceptable and potential ramifications for unprofessional behavior. https://science.osti.gov/SW-DEI/DOE-Diversity-Equity-and-Inclusion-Policies/Harassment
- **How to Address or Report Behaviors of Concern**– Process on how and who to report issues, including the distinction between reporting on unprofessional, disrespectful, or disruptive behaviors, and behaviors that constitute a violation of Federal civil rights statutes. https://science.osti.gov/SW-DEI/DOE-Diversity-Equity-and-Inclusion-Policies/How-to-Report-a-Complaint
- **Implicit Bias** – Be aware of implicit bias, understand its nature – everyone has them - and implicit bias if not mitigated can negatively impact the quality and inclusiveness of scientific discussions that contribute to a successful meeting. https://kirwaninstitute.osu.edu/article/understanding-implicit-bias

U.S. DEPARTMENT OF ENERGY | Office of Science

Our Mission:

Deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States.

More than **34,000 r**esearchers supported at more than **300** institutions and **17** DOE national laboratories

Steward **10** of the 17 DOE national laboratories

More than **37,000** users of **28** Office of Science scientific user facilities

$8.1B
(FY 23 enacted)

OFFICE OF SCIENCE BY THE NUMBERS

Delivering scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States

FY23

6 CORE SCIENCE PROGRAMS

- Advanced Scientific Computing Research
- Basic Energy Sciences
- Biological and Environmental Research
- Fusion Energy Sciences
- High Energy Physics
- Nuclear Physics

3 ENGINEERING AND TECHNOLOGY OFFICES

- Accelerator Research and Development and Production
- Isotope Research and Development and Production
- Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)

5 NATIONAL QUANTUM INFORMATION SCIENCE RESEARCH CENTERS

ACROSS ITS 10 NATIONAL LABS, OFFICE OF SCIENCE MAINTAINS APPROXIMATELY

24 MILLION SQUARE FEET OF SPACE

1,600 BUILDINGS

38,000 ACRES OF LAND OWNED

SUPPORTS RESEARCH SPANNING

16 DOE NATIONAL LABS

50 STATES, GUAM, PUERTO RICO, AND WASHINGTON, D.C.

>310 UNIVERSITIES AND HIGHER-LEARNING INSTITUTIONS

4 BIOENERGY RESEARCH CENTERS

2 ENERGY INNOVATION HUB PROGRAMS

51 ENERGY FRONTIER RESEARCH CENTERS

STEWARDS 10 DOE NATIONAL LABORATORIES

3 World-Leading Supercomputers

ESTIMATED RESEARCHERS SUPPORTED

- **11,100** Permanent PhDs
- **3,400** Postdoctoral Associates
- **5,200** Graduate Students
- **9,700** Other Scientific Personnel

OVER 39,500 USERS AT 28 OFFICE OF SCIENCE FACILITIES

10 SITE OFFICES

1 CONSOLIDATED SERVICE CENTER

OVER 100 NOBEL PRIZES

$8.1 BILLION OVERALL OFFICE OF SCIENCE BUDGET

$918 MILLION USER FACILITY CONSTRUCTION

$281 MILLION SCIENCE LABORATORIES INFRASTRUCTURE

The Office of Science Research Portfolio

Advanced Scientific Computing Research	• Delivering world leading computational and networking capabilities to extend the frontiers of science and technology
Basic Energy Sciences	• Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
Biological and Environmental Research	• Understanding complex biological, earth, and environmental systems
Fusion Energy Sciences	• Supporting the development of a fusion energy source and supporting research in plasma science
High Energy Physics	• Understanding how the universe works at its most fundamental level
Nuclear Physics	• Discovering, exploring, and understanding all forms of nuclear matter
Isotope R&D and Production	• Supporting isotope research, development, production, processing and distribution to meet the needs of the Nation
Accelerator R&D and Production	• Supporting new technologies for use in SC's scientific facilities and in commercial products

ASCR Office Hours

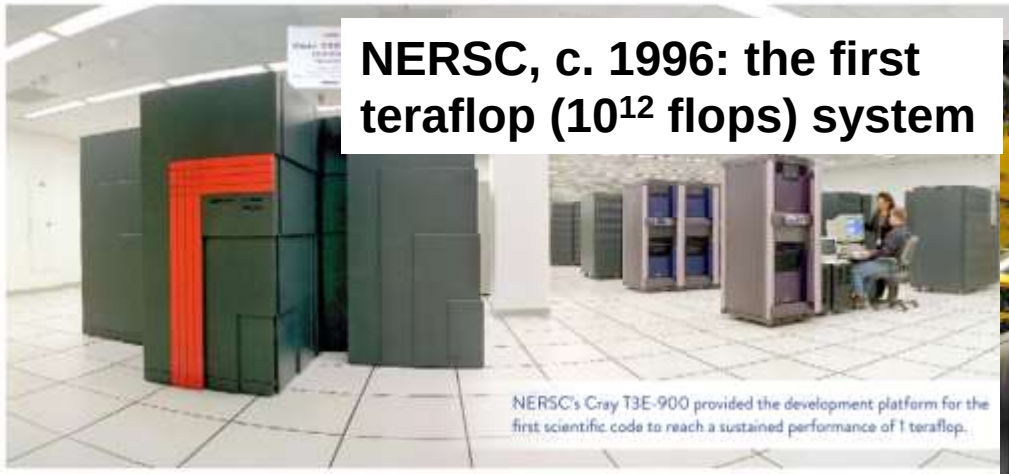
- Starting in March, ASCR started holding virtual office hours on the second Tuesday of the month, 2 PM ET
- Researchers, educators, and leaders within research administration from all institutional types are encouraged to join
- A primary goal of the virtual office hours is to broaden awareness of our programs; no prior history of funding from DOE is required to join
- Program managers are available to answer questions
- Past topics:
  - *Tuesday, March 12, 2024, at 2pm ET – Introduction to ASCR and its program mission and history*
  - *Tuesday, April 9, 2024, at 2pm ET – Introduction to ASCR's Computer Science research program*
  - *Tuesday, May 14, 2024, at 2pm ET – Introduction to ASCR's Applied Mathematics research program*
  - *Tuesday, June 11, 2024, at 2pm ET – Introduction to ASCR's user facilities and their allocation programs*
  - *Tuesday, July 9, 2024, at 2pm ET – Overview of the ASCR research proposal and review process*
- Current topic:
  - *Tuesday, August 13, 2024, at 2pm ET – Introduction to the Scientific Discovery through Advanced Computing (SciDAC) research program*

See the ASCR website (https://science.osti.gov/ascr/officehours) for more information, including slides and recordings of past office hours.

ASCR – over 70 years of Advancing Computational Science

Beginnings: During the Manhattan Project, John Von Neumann advocated for the creation of a Mathematics program to support the continued development of applications of digital computing

Over 40+ years, ASCR has a rich history of investment in computational science and applied mathematics research, and revolutionary computational and network infrastructure.



NERSC, c. 1996: the first teraflop (10^{12} flops) system

Today, Frontier at OLCF: first to exascale (10^{18} flops)

WHY COMPUTATIONAL SCIENCE?

- Computational science adds a third pillar to researcher's toolkit along side theory and experiments
- Computational science is essential when experiments are too expensive, dangerous, time-consuming or impossible
- Computational science facilitates idea-to-discovery that leads from equations to algorithms
- Virtually every discipline in science and engineering has benefited from DOE's sustained investments in computational science

SciDAC (Scientific Discovery through Advanced Computing)

- **SciDAC** is an Office of Science Program that was initiated in 2001 as an SC-wide program to dramatically accelerate progress in scientific discovery via advanced computing and includes:
- **SciDAC Institutes** – sponsored by ASCR & participate in partnerships
- **SciDAC Partnerships** across SC- span the SC Science Programs via partnerships with ASCR
- **SciDAC Partnerships** between ASCR and some of the DOE Applied Offices
- The SciDAC research community consists of scientists, applied mathematicians, and computer scientists, from various subdisciplines, representing multiple DOE national laboratories, multiple universities, and industry and holds an annual PI meeting to exchange results and ideas.
- The SciDAC program has been recognized as a leader in enabling scientific discoveries that would not have been possible without the strong collaborations between discipline scientists, applied mathematicians, and computer scientists.
- While SciDAC 1 in 2001 focused on Terascale computing, the current cycle of SciDAC 5 advances scientific discovery at Exascale (see next slide)
- More information can be found at https://www.scidac.gov

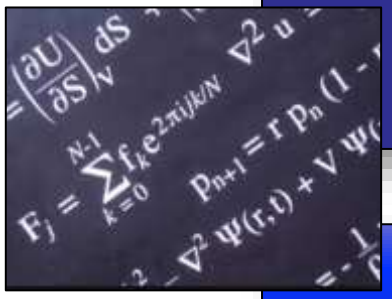
SciDAC over the Years

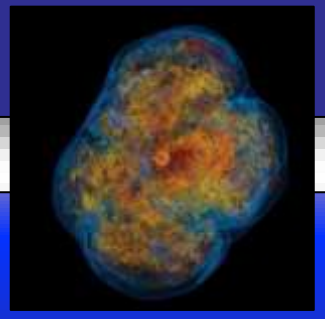
Program	Time Frame	Description	Result
SciDAC-1	2001 – 2006	Created scientific software infrastructure for parallel computing; Funded collaborations in DOE science domains	Science at the Terascale
SciDAC-2	2006 – 2011	Added DOE science domains; Enhanced university involvement; Outreach to broader scientific community; Added Data & Visualization	Science to the Petascale
SciDAC-3	2011 – 2016	Improved collaborations among the Institutes and between ASCR-SC programs; Enhanced architecture- and applications-awareness within each Institute; Added Uncertainty Quantification	Science on multi-core and emerging hybrid architectures
SciDAC-4	2017 - 2021	Outreach to broader scientific community; First connection to Applied Energy; Built-in flexibility; Added Machine Learning	Science on pre-exascale architectures
SciDAC-5	2020 - 2027	SciDAC refocused on introducing new AI and ML algorithms and tools. Added pilot program with the Office of Electricity.	Science at the Exascale

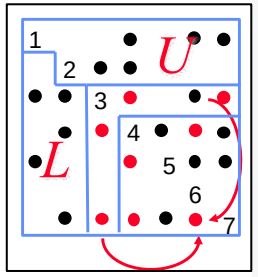
FASTMath focuses on leading edge applied/computational mathematics in SciDAC

Develop robust math techniques and numerical algorithms for DOE science problems

- Eight focused topical areas based on application needs
- AI/ML cross-cutting across all areas
- High-level synergistic techniques







Work closely with domain scientists to leverage our math and ML expertise and deploy our software in large-scale scientific codes

- Build from existing connections with basic research
- Focus on research results that are most likely to meet application needs

FASTMath

Provide leading edge applied and computational mathematics to remove the barriers facing computational scientists

Deliver highly performant software with strong software engineering to run efficiently and scalably on DOE supercomputers

- Algorithmic and implementation scalability
- Performance portability
- Interoperability of libraries

Build and support the broader computational math and computational science communities across DOE

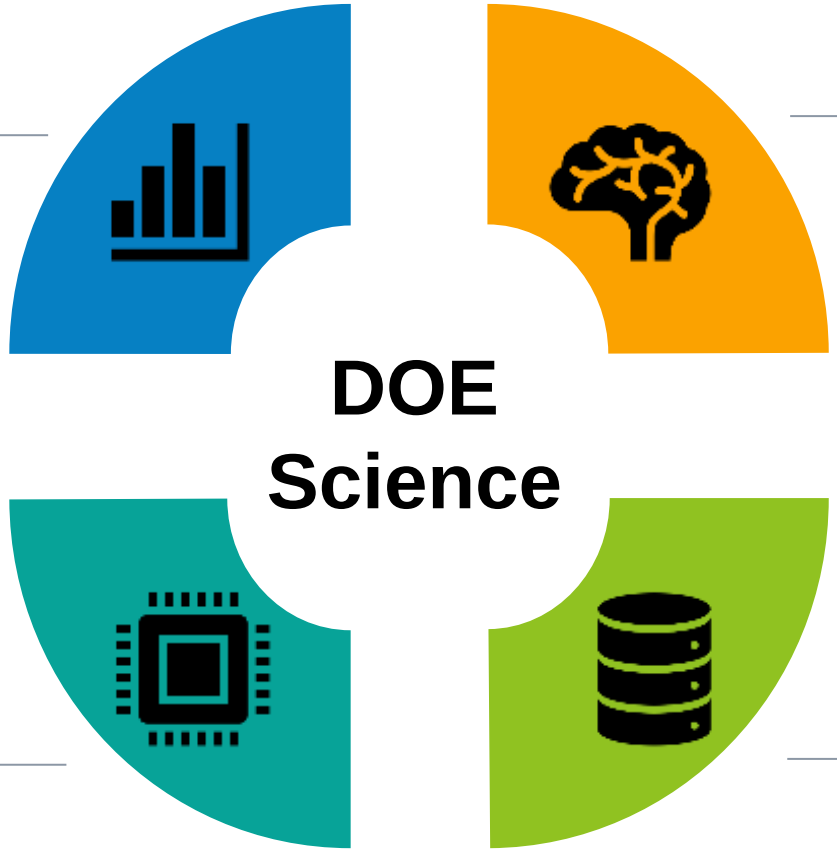
- Publications and presentations in highly visible venues
- Team tutorials
- Workforce pipeline and training
- Web presence

RAPIDS2 targets key computer science needs in four areas

RAPIDS

Data Understanding

- Ensemble analysis
- Feature detection
- Production visualization
- In situ analysis



Artificial Intelligence

- Representation learning
- Surrogate modeling
- Automation

Platform Readiness

- Heterogeneous programming
- Autotuning
- Performance modeling and analysis
- Correctness

Scientific Data Management

- Storage and I/O
- Data Reduction
- Knowledge management
- Workflow automation

Program Manager: Kalyan Perumalla (ASCR)

SciDAC Partnerships across Office of Science & DOE

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Basic Energy Sciences	• Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
Biological and Environmental Research	• Understanding complex biological, earth, and environmental systems
Fusion Energy Sciences	• Supporting the development of a fusion energy source and supporting research in plasma science
High Energy Physics	• Understanding how the universe works at its most fundamental level
Nuclear Physics	• Discovering, exploring, and understanding all forms of nuclear matter
DOE Office of Nuclear Energy	Office of Nuclear Energy | Department of Energy
DOE Office of Electricity	Office of Electricity | Department of Energy

BES-ASCR SciDAC Partnership Re-competed in FY 2021

Scientific Discovery through Advanced Computing: Partnerships in Basics Energy Sciences DE-FOA-0002441 FOA Issue Date: Dec 9, 2020

The announcement sought for integrated teams will engage with the SciDAC Institutes and DOE HPC computing capabilities. Two topical areas of interest were targeted:

Quantum Phenomena of many-particle systems driven far from equilibrium. Applications are sought that drive and manipulate quantum effects such as coherence, entanglement, and novel states of matter by going beyond the use of existing quantum-based methods in their traditional regimes.

Predictive Control of Reaction Pathways for chemical mechanisms in complex nonequilibrium and field-driven environments important in synthesis of materials and chemicals, and deconstruction of macromolecular structures such as plastics for polymer upcycling. Efforts aimed at extending currently attainable length/time scales or increasing complexity and that algorithmically match efficiency enhancements offered by next generation computers will receive priority.

Awards made are listed at: https://scidac.gov/partnerships/basic-energy-sciences.html

Program Managers: Matthias Graf (BES) & Marco Fornari (ASCR)

BER-ASCR SciDAC Partnership Re-competed in FY 2022

Scientific Discovery through Advanced Computing: Partnerships in Earth System Model Development DE-FOA-0002585 FOA Issue Date: Nov 22, 2021

- The DOE SC programs in Biological and Environmental Research (BER) and Advanced Scientific Computing Research (ASCR) announce their interest in receiving applications from multi-disciplinary teams to establish collaborative projects under the SC-wide Scientific Discovery through Advanced Computing (SciDAC) program in specific targeted topic areas that relate to the BER and ASCR missions.
- Exploit the capabilities of DOE high-performance computing (HPC) in order to accelerate and enhance the DOE's Energy Exascale Earth System Model (E3SM) development.
- This SciDAC opportunity targets current challenges of the E3SM to improve its representations and performance of the Atlantic Meridional Ocean Circulation (AMOC), the Antarctic ice sheet, marine biogeochemistry, and quasi-biennial oscillation (QBO), as well as improved physics and numerics to enhance coupling of the various components with high and variable resolutions of the E3SM.

Biological and Environmental Research | Scientific Discovery through Advanced Computing (scidac.gov)

Program Managers: Xujing Davis (BER) & Lali Chatterjee (ASCR)

FES-ASCR SciDAC Partnership Recompeted in FY2023

- **SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING (SCIDAC) –**

  FES PARTNERSHIPS. DE-FOA-0002924 Issue Date: March 8, 2023

- Enable or accelerate scientific discovery and programmatic objectives, aligned with the FES mission and the Department's vision for fusion energy (https://www.whitehouse.gov/ostp/news-updates/2022/04/19/readout-of-the-white-house-summit-on-developing-a-bold-decadal-vision-for-commercial-fusion-energy/)
- Effective collaborations between fusion / plasma scientists and applied mathematicians and/or computer scientists from the SciDAC Institutes (https://www.scidac.gov/institutes.html) that fully exploit the capabilities of DOE High Performance Computing (HPC) facilities.
- Focus on Whole facility modelling

Awards can be viewed at: https://scidac.gov/partnerships/fusion-energy.html

Program Managers: Michael Halfmoon (FES) & Lali Chatterjee (ASCR)

HEP-ASCR SciDAC Partnership Recompeted in FY 2022

SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING: HIGH ENERGY PHYSICS

DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 22-2580 –Issued Nov 3, 2021

Enable or accelerate scientific discovery aligned with the HEP mission by productive collaborations between high energy physicists, and applied mathematicians and computer scientists from the SciDAC Institutes in order to fully exploit the capabilities of DOE HPC. Focus:

- Integrated end-to-end simulation of conventional, hybrid, or "virtual" accelerators using DOE HPC to target Grand Challenges to advance the P5 Science Drivers
- Novel detector simulation and tracking models and data driven analysis techniques for high energy physics experiments employing DOE HPC.
- Innovative theoretical, computational, and simulation techniques to explore the unknown including new particles, interactions, and physical principles.

[High Energy Physics | Scientific Discovery through Advanced Computing (scidac.gov)]

Program Managers: Jeremy love (HEP) and Lali Chatterjee (ASCR)

NP-ASCR SciDAC Partnership Recompeted in FY 2022

SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING (SCIDAC): PARTNERSHIP IN NUCLEAR PHYSICS DE-FOA-0002589 Issue Date: December 22, 2021

The NP mission is "to discover, explore, and understand all forms of nuclear matter." Focus areas of the FOA included:

Precision studies of meson and baryon spectra, including exotic states of QCD, and their decays and photo couplings

Properties and interactions of light nuclei and multi-nucleon systems

Precision calculations of nuclear matrix elements for fundamental symmetries

Neutrino and electron interactions in nuclei and dense matter

Nuclear tomography at femtometer scale: 3-D spatial imaging of nucleons and inferring quantum correlations of quarks and gluons inside the nucleon

Nuclear structure and properties of nuclei; Nuclear reactions, microscopic models, fission, and nucleosynthesis

Properties of quark-gluon plasma; QCD equation of State

https://scidac.gov/partnerships/nuclear-physics.html

Program Managers: Xiaofeng Guo (NP) and Lali Chatterjee (ASCR)

NE-ASCR SciDAC Partnership Re-competed in FY 2022

SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING (SCIDAC): PARTNERSHIP IN NUCLEAR ENERGY, DE-FOA-0002592 FOA Issue Date: Dec 14, 2021

- The NE mission (https://www.energy.gov/ne/about-us) encourages the development and exploration of advanced nuclear science and technology.

- Current award: "Simulation of the Response of Structural Metals in Molten Salt Environment"
- Previous award: "Simulation of Fission Gas in Uranium Oxide Nuclear Fuel"

In each case, original research in applied mathematics has been required to enable the original research related to nuclear energy.

Program Managers: David Henderson (NE) & David Rabson (ASCR)

OE-ASCR SciDAC Partnership inaugural solicitation FY24, in review

SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING (SCIDAC): PARTNERSHIP IN ELECTRICITY, LAB 24-3310, May 7 2024

- The DOE Office of Electricity (OE, https://www.energy.gov/oe/about-office-electricity) provides national leadership to ensure that the nation's energy-delivery system is secure, resilient, and reliable.

- Current pilot project: "Space Weather Mitigation Planning"
- Current pilot project: "Probabilistic Impact Scenarios for Extreme Weather Event Resilience"

Program Managers: Alireza Ghassemian (OE) & David Rabson (ASCR)

Performance portability solutions for GPUs and CPUs to track reconstruction kernels

with the SciDAC-HEP NeuCol partnership

Scientific Achievement

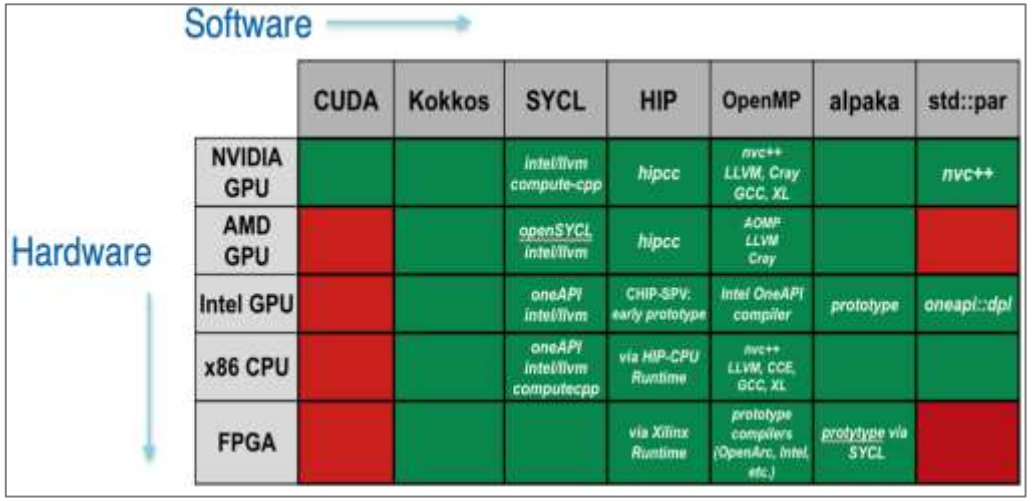
We ported two mini-apps (p2z and p2r) from the mkFit application in the Compact Muon Solenoid (CMS) software framework to different CPUs and GPUs using various performance portability solutions and found the best mapping strategies to achieve the performance portability across diversely heterogeneous target systems.

Significance and Impact

High Energy Physics (HEP) experiments confront computing challenges from increasing detector sizes and accelerator intensities. The Compact Muon Solenoid (CMS) detector at the CERN LHC will face a factor of ~20 increase in reconstruction CPU time from the High-Luminosity LHC (HL-LHC) upgrade. Therefore, developing portable accelerator versions of the HEP application will be able to accelerate the software-based High-Level Trigger (HLT) across heterogeneous systems.

Technical Approach

- Ported two important mini-apps (p2z) and p2r) to CPUs and GPUs using various programming models (Kokkos, SYCL, C++17 std::execution::par, Alpaka, OpenMP, and OpenACC).
- Studied the performance of these mini-apps on the tested CPUs and GPUs and found the best parallelism and data mapping strategies.



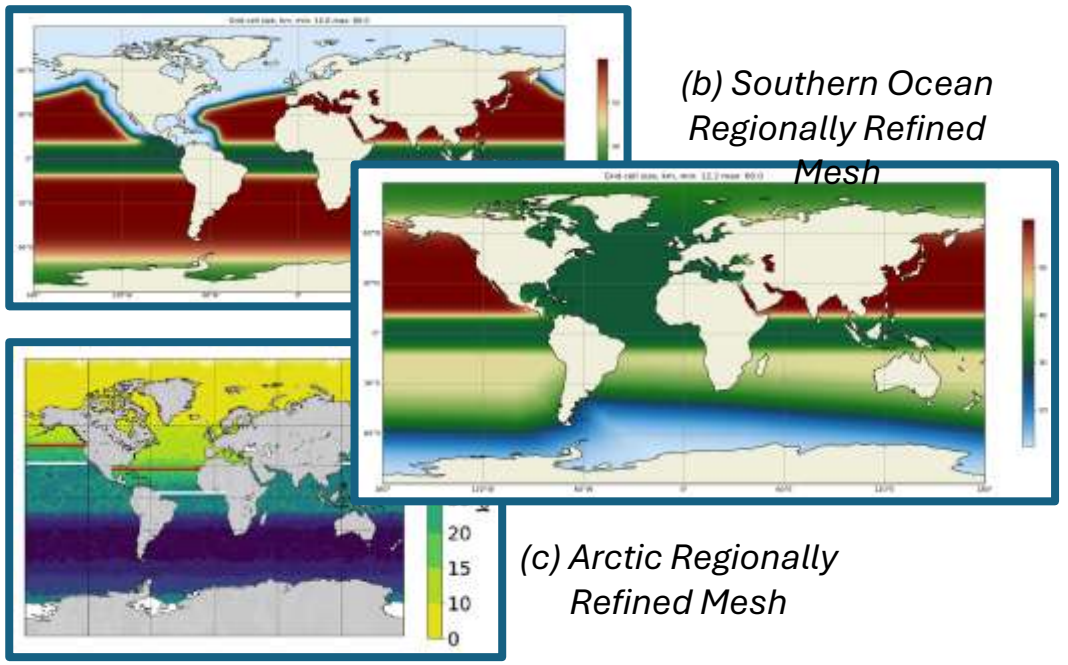
Summary of hardware supports for different portability solutions*. Green indicates officially supported, red indicates unsupported.*
We applied these portability solutions on two mini-apps (p2z and p2r) extracted from the HEP application called mkFit and evaluated these portability solutions, in terms of the development efforts and their performance on GPUs and many-core CPUs from different vendors (Intel, AMD, NVIDIA).

PI(s): Robert Ross (ANL); Local Lab POC: Seyong Lee (ORNL)
Collaborating Institutions: ORNL, FNAL, United States Naval Academy, Cornell University, University of Oregon
ASCR Program: SciDAC RAPIDS2 ASCR PM: Kalyan Perumalla
Publication for this work: K. H. M. Kwok, et al., "Application of performance portability solutions for GPUs and many-core CPUs to track reconstruction kernels", *International Conference on Computing in High Energy & Nuclear Physics (CHEP), 2023.*

Seahorce: First Look into Testing the Limits/Capabilities of MPAS-O's Ultra-High Coastal Regional Refinement Capabilities

(a) North American Regionally Refined Mesh

(b) Southern Ocean Regionally Refined Mesh



(c) Arctic Regionally Refined Mesh

Veneziani et al (2022)

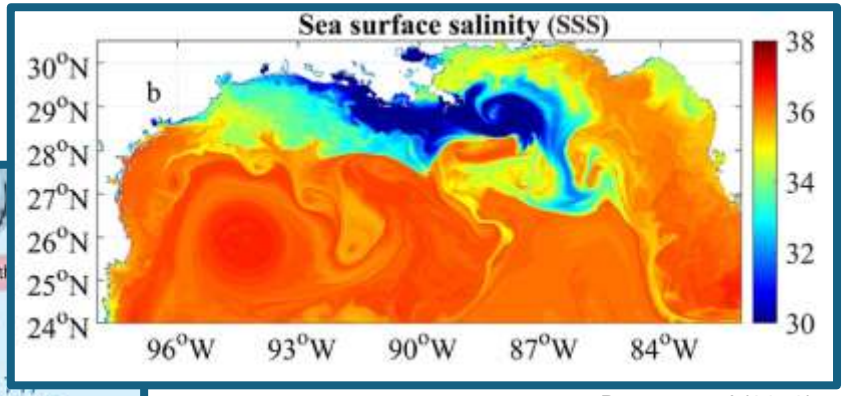
Figure 1. Examples of MPAS-O Regional Refinement meshes for (a) the North American Coast, (b) the Southern Ocean, and (c) the Arctic Ocean.

What are the limits of the regional refinement capability within E3SM?

And what developments can be done to enable ultra-high-resolution simulations of coastal regions?

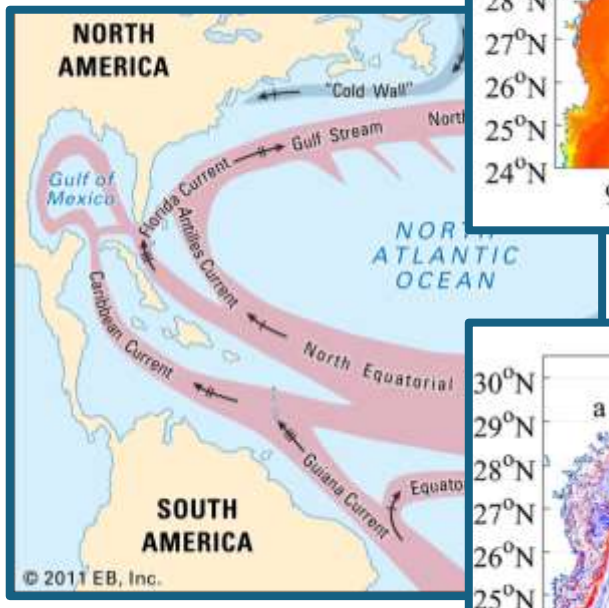
Northern Gulf of Mexico Test Region

(a) Sea Surface Salinity



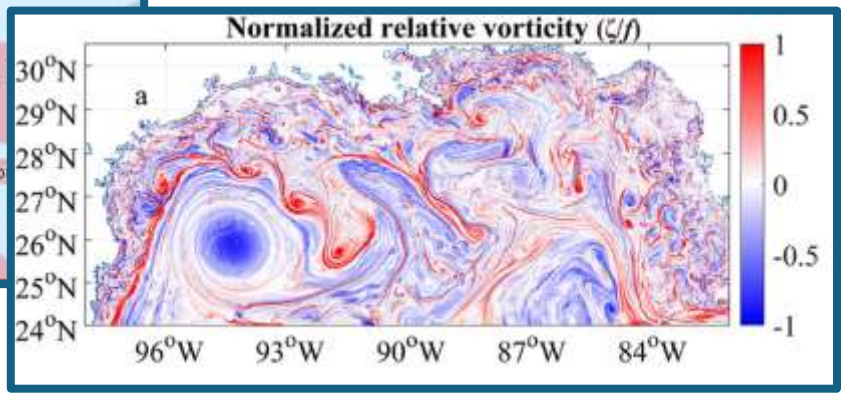
Bracco et al (2019)

(c) Large scale circulation



Encylopedia Britannica, Inc.

(b) Surface vorticity field



Bracco et al (2019)

Figure 2. Northern GoM test region with (a) strong river freshwater runoff, (b) rich small-scale eddy features, and (c) connections to the larger-scale Atlantic and global circulations.

High-Order Remapping from MPAS-Ocean to ROMS

With the SEAHORCE Partnership (BER)

Scientific Achievement

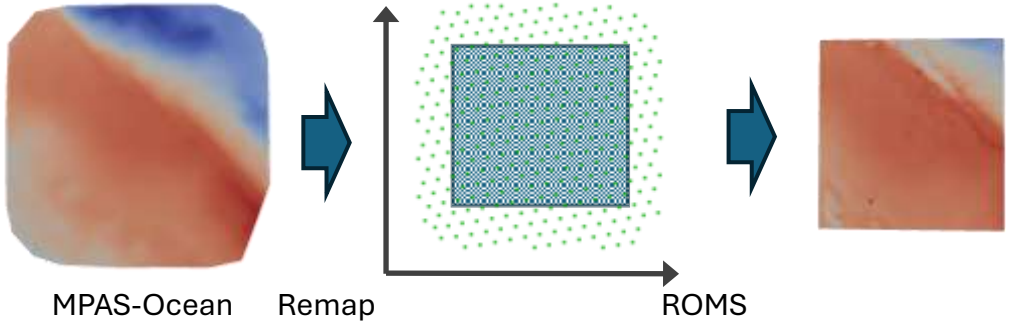
Oceanographic data are accurately transferred from a coarse global climate simulation (MPAS-Ocean) to a high-fidelity regionally-refined simulation (ROMS) through the use of Multivariate Functional Approximation (MFA).

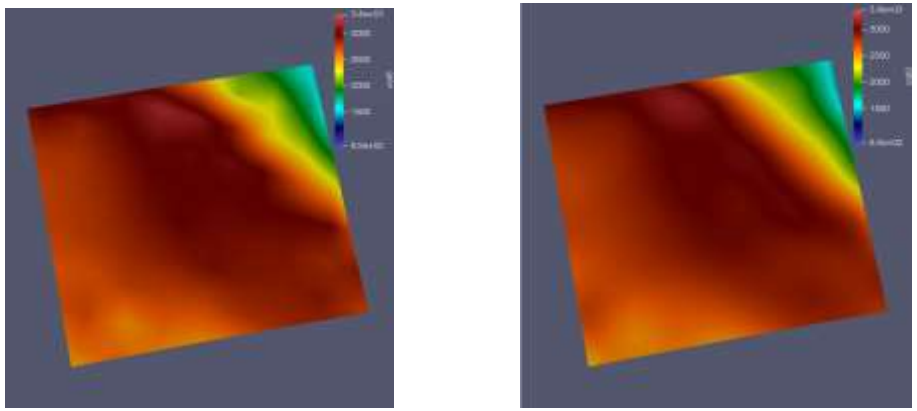
Significance and Impact

MFA provides a high-order intermediate representation to smoothly transform 3D fields between two simulations, producing consistent, high-order accurate, and smooth downsampled fields from coarse MPAS-O to **10X** finer ROMS meshes. The continuous MFA model can enable multiscale coupling while preventing mesh artifacts that result from intersection-based conservative L_2 projections.

Technical Approach

- MFA is a meshless data representation built on a B-spline functional model.
- Any mesh-based data set may be converted into an MFA model, and subsequently converted back to a different mesh structure.
- Field remapping is achieved by representing coarse mesh data produced by MPAS-Ocean as an MFA model, then resampling the model on the fine mesh used by ROMS.





Top row: Data produced by MPAS-Ocean (left) on a coarse (green) mesh are remapped to a fine (blue) mesh that can be used as input to ROMS (right). Bottom row: Controlling the degree of smoothness using MFA. Bathymetry in MPAS is remapped to ROMS, with the polynomial degree=1 (left) compared with degree=3 (right). The scientist can accentuate high-frequency details or low-frequency overall trends by selecting the MFA degree. The MFA library was developed under ASCR ECRP and is maintained under the SciDAC RAPIDS Institute.

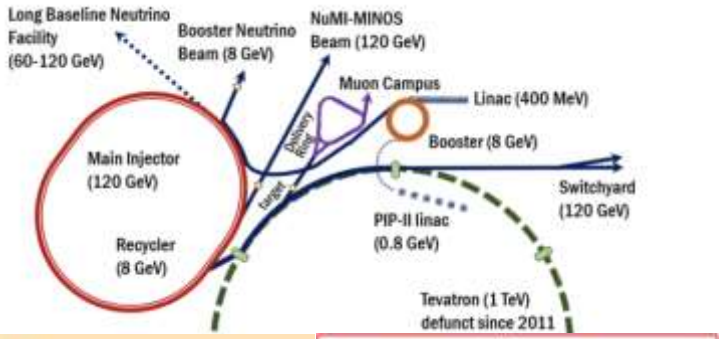
PI(s)/Facility Lead(s): Tom Peterka, David Lenz, Vijay Mahadevan (ANL)
Collaborating Institutions: Argonne National Laboratory
ASCR Program: SciDAC
ASCR PM: Kalyan Perumalla
Publication(s) for this work: Lenz et al. Customizable Adaptive Regularization Techniques for B-Spline Modeling. Journal of Computational Science, 71, 2023.
Code Developed: https://github.com/tpeterka/mfa

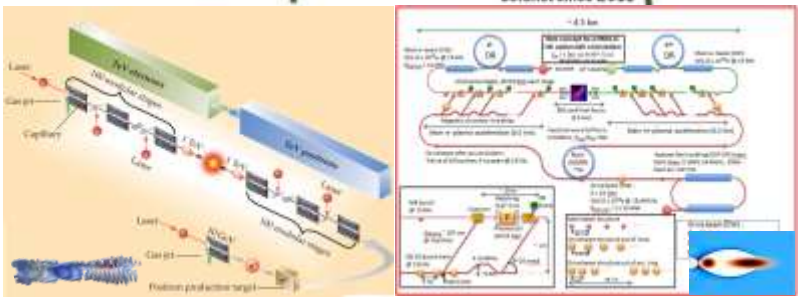
SciDAC
Scientific Discovery through Advanced Computing

HEP

Collaboration for Advanced Modeling of Particle Accelerators

Fermilab SLAC NATIONAL ACCELERATOR LABORATORY
CAMPA
UCLA
Argonne NATIONAL LABORATORY
OAK RIDGE National Laboratory





Science thrusts

a) Fermilab complex: PIP-II+booster.
b) design of plasma-based colliders.

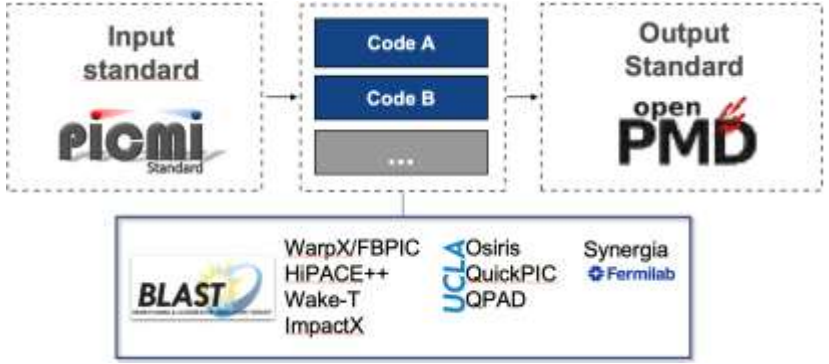
Team

BERKELEY LAB — PIC algorithms & WarpX Code, Plasma Modeling
FASTMATH — AMReX, Solvers
Fermilab, UCLA — Conventional/Plasma Accelerator Modeling
SLAC, Argonne, FASTMATH, OAK RIDGE National Laboratory, RAPIDS — AI/ML, Optimization Data I/Os

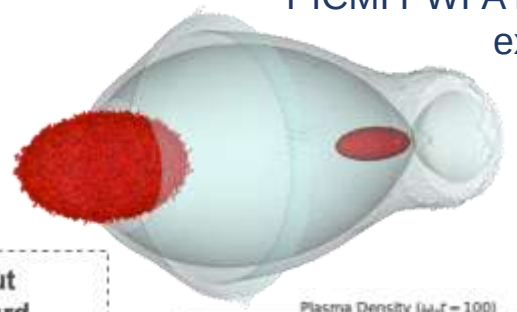
Thrusts

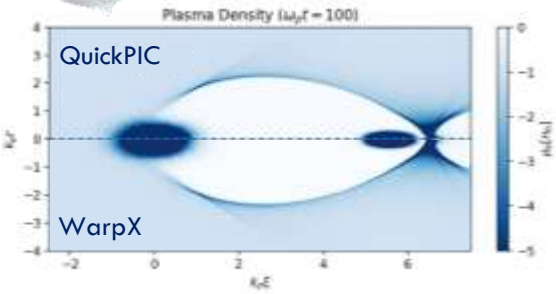
Computational Thrusts

a) Codes readiness for GPUs
b) Algorithmic innovation
c) Integrated ecosystem
d) Toward digital twins



PICMI PWFA FACET example using ~same PICMI input script



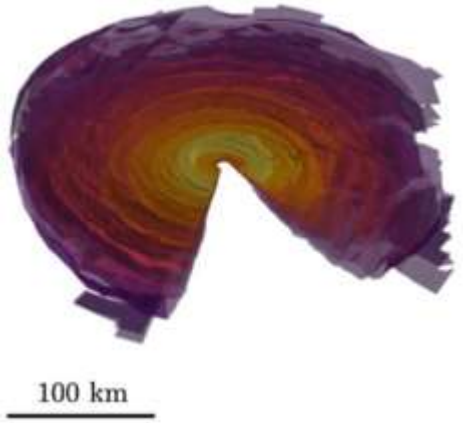


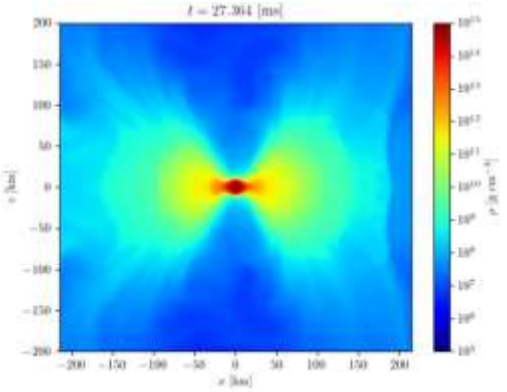
Some NP-ASCR SciDAC Partnership Simulations

Neutron Star Merger Simulations

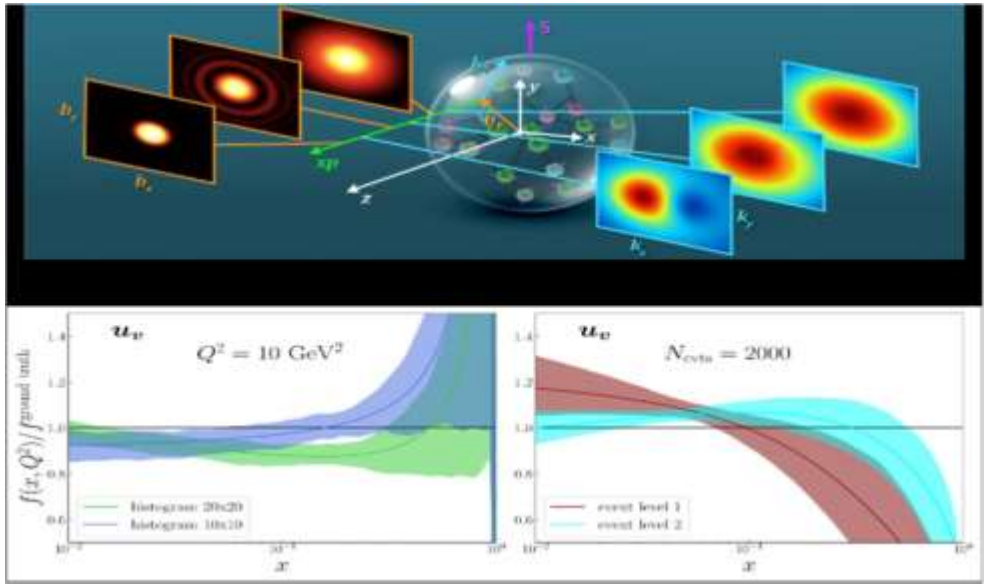
Accomplishment: Performed 44 general-relativistic neutron star merger simulations with neutrinos and turbulent viscosity; Discovered that disks' specific angular momentum, entropy, and composition depend weakly on binary properties

Impact: Provided fits to construct realistic disk profiles for long-term post-merger simulations and nucleosynthesis studies





Camilletti et al., PRD109, 063023 (2024)



3-D Imaging of quark-gluon structure inside a proton:

- Framework demonstrated for the analysis of deep inelastic scattering data at the event level !
- Next step to include a surrogate detector model with full end-to-end analysis

SciDAC
Scientific Discovery through Advanced Computing

FES

Kinetic IFE Simulations at Multiscale with Exascale Technologies

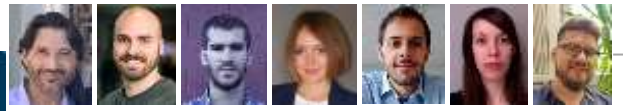
KISMET

WarpX

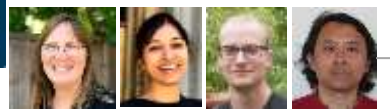
Two Computational Thrusts

a) Particle-In-Cell algorithms & WarpX
b) Scalable data visualization & analysis

Team



PIC algorithms & WarpX Code, Plasma Modeling



AMReX, Solvers

Target Surface & Hotspot Physics, Implicit Solvers

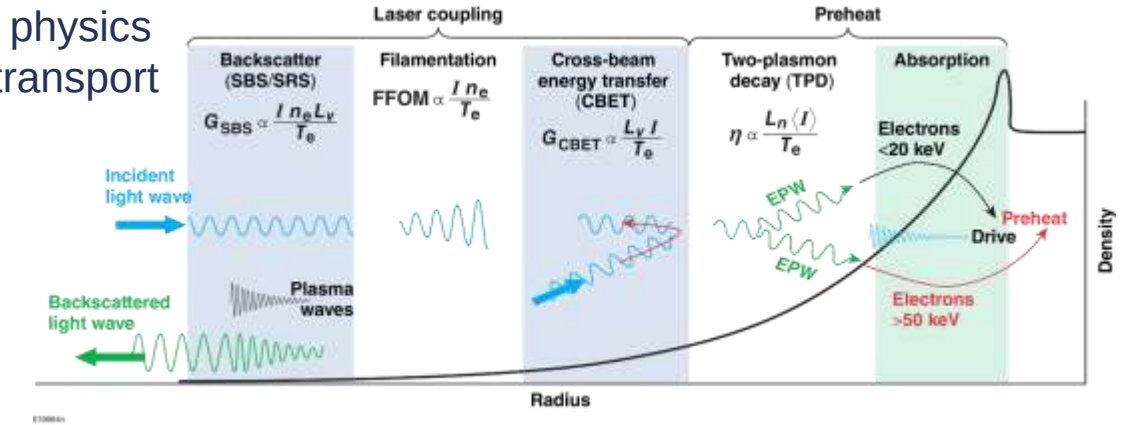
Low Density Plasma Physics, Laser Absorption & Transport

Data Visualization & Analysis

Thrusts

Four Physics Thrusts (aligned with 2023 IFE BRN)

a) low-density plasma physics
b) laser absorption & transport
c) target surface
d) hotspot physics



Development of a Robust Implicit Electromagnetic Gyrokinetic PIC Algorithm

This FES-ASCR collaborative work was performed at LANL (led by L. Chacón) and PPPL as part of the SciDAC-4 HBPS activities (PI, C.S. Chang)

Scientific Achievement

- Explicit electromagnetic algorithms used in the fusion 5D gyrokinetic PIC codes, such as XGC, often experience numerical
  - finite-grid instabilities or
  - CFL type instabilities when Alfven frequency is high
- A new implicit time-stepping scheme that is specifically developed for 5D gyrokinetic PIC algorithm has removed these issues.

Significance and Impact

Enables a highly robust tool for electromagnetic gyrokinetic PIC simulations of fusion reactor plasmas that will significantly reduce exascale computing cost by avoiding numerical instabilities

Research Details

- A fully implicit method with carefully chosen discrete formulation including strict conservations has enabled stable simulations over a large range of physical and numerical parameters relevant to fusion reactors
- An optimized fluid-based preconditioner has facilitated an efficient iterative solution method with performance that is insensitive to Alfven frequency and CFL parameters

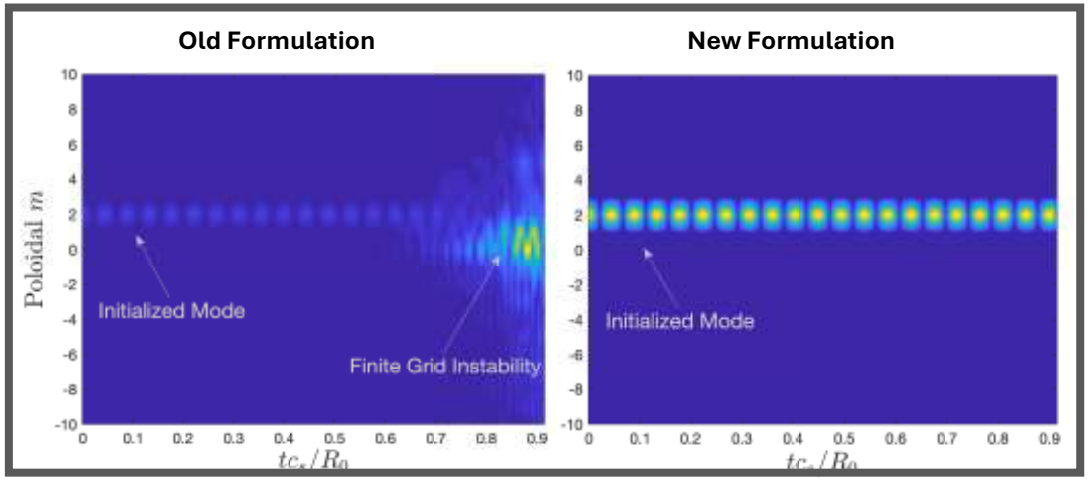


FIG. Robustness of the new implicit gyrokinetic scheme: Shear Alfvén waves are excited from an initial perturbation in XGC. With the usual implicit/explicit formulation (left), the finite-grid instability, characterized by long wavelengths in the poloidal plane, quickly develops. The new implicit formulation (right) allows for clean, numerically stable simulations in XGC.

Work completion based on previous HBPS publications

B. Sturdevant et al., *Phys. Plasmas* 28, 072505 (2021)
B. Sturdevant and L. Chacón, *J. Comp. Phys.* 464, 111330 (2022)

HBPS

U.S. DEPARTMENT OF ENERGY | Office of Science

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Los Alamos NATIONAL LABORATORY

Flash-X Performance Orchestration [RAPIDS with NP SciDAC]

We started developing an end-to-end performance portability solution for Multiphysics applications under the Exascale Computing Project. The solution is language agnostic, obviating the need to rewrite the code in C++ as most other solutions do. The solution is now deployed in Flash-X for some of the physics.

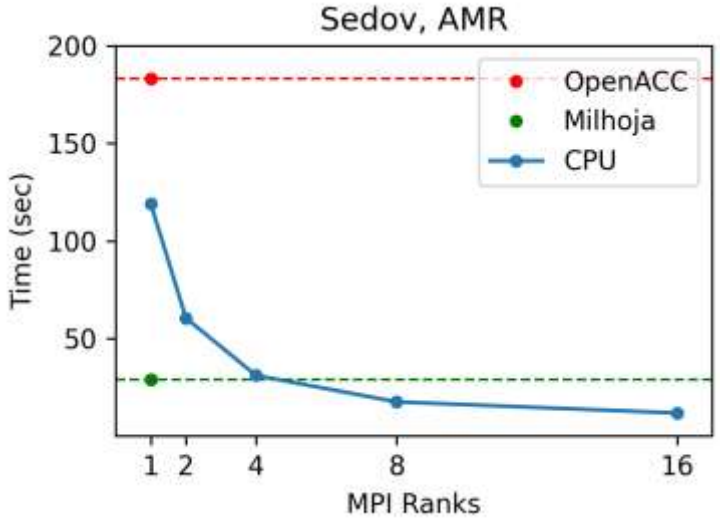
Significance and Impact

- Our approach provides an effective solution that is designed to evolve with the evolution of hardware and software complexity. It can be applied to many legacy codes also.
- Some of our tools provide complimentary features to existing C++ solutions, and therefore can be used in combination with those solutions.

Technical Approach

. It uses three sets of tools, each one addressing one aspect of performance.

- **Unify expression of arithmetic with different data layouts for different devices**: This is done with macros that can have multiple alternative definitions, and a tool that can arbitrate on selecting the most suitable one.
- **Unify algorithmic variants and map computation to devices**: Algorithmic variants are expressed in pseudocode like recipes specifying order of execution and where to execute which computation.
- **Move data and computation to targets specified in the recipe**. This is done with a domain specific runtime Milhoja. The code to interface with Milhoja is also generated along with recipe translation.



This figure shows performance comparison of using shock hydrodynamics with adaptive mesh refinement in three different modes. The top dotted line is the performance using OpenACC offloading within a block, and the bottom green lines shows offloading done with our toolchain. The solid blue line is CPU only performance..

PI(s)/Facility Lead(s): Person Name; Anshu Dubey
Collaborating Institutions: Virgina Tech, Riken
ASCR Program: [ECP, SciDAC.]
ASCR PM: Lali Chatterji, Kalyan Perumalla
Publication(s) for this work : Youngjun, et al., in preparation
Dubey et al., https://doi.org/10.1016/j.future.2023.07.014
O'Neal et al, https://doi.org/10.1007/978-3-031-06156-1_13

ENAF Exascale Nuclear Astrophysics for FRIB

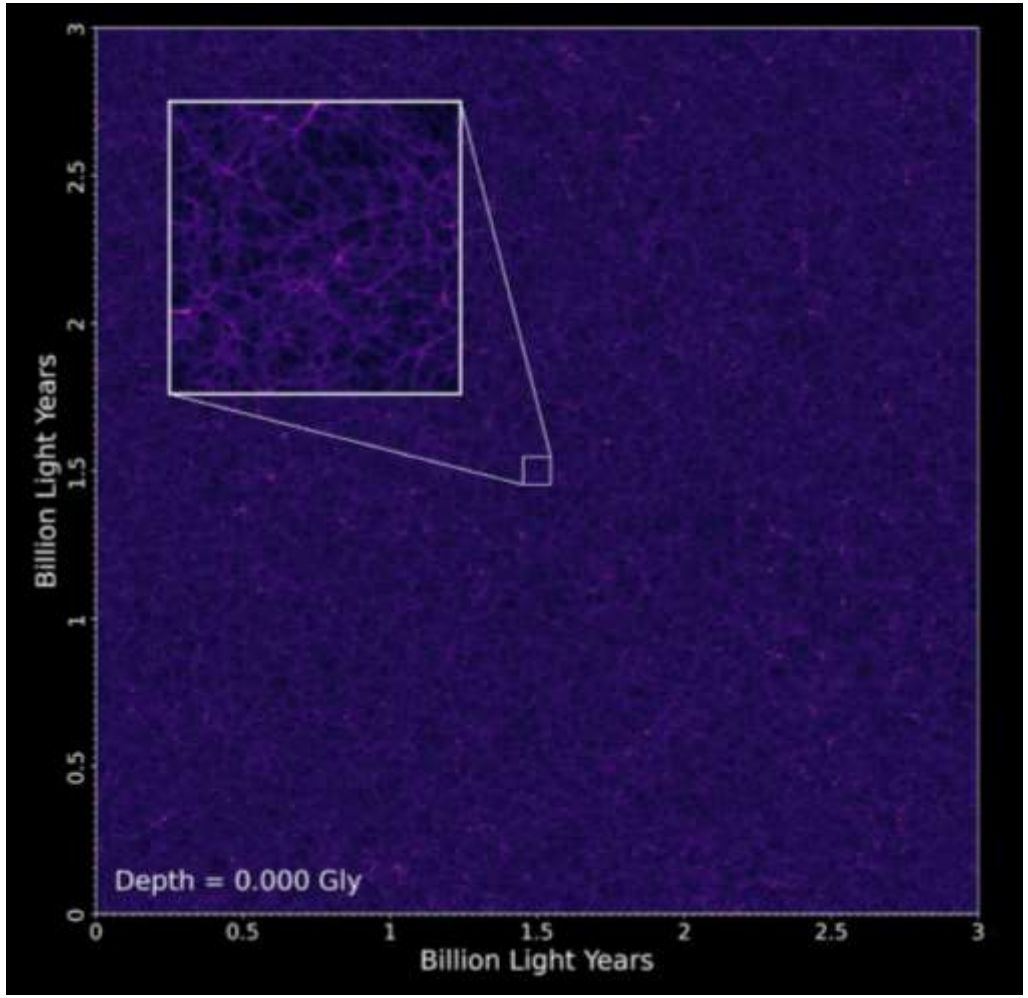
VIRGINIA TECH

RIKEN R-CCS RIKEN Center for Computational Science

Argonne NATIONAL LABORATORY

Correlated sky from HACC and Nyx

- Different cosmological probes from the Dark Energy Spectroscopic Instrument (DESI) require different simulation approaches
- Our codes, HACC & Nyx, offer the unique opportunity of modeling the same sky, combining theirs strengths to capture different probes, here galaxy clustering and the Lyα forest
- We produced a Nyx simulation to reconstruct accurate Lyα forest combined with a high-resolution HACC simulation to capture halos/galaxies/quasars in the same volume
- The volume is ~1000 larger than state-of-the-art Lyα simulations leading to the first realistic DESI mock across redshifts!

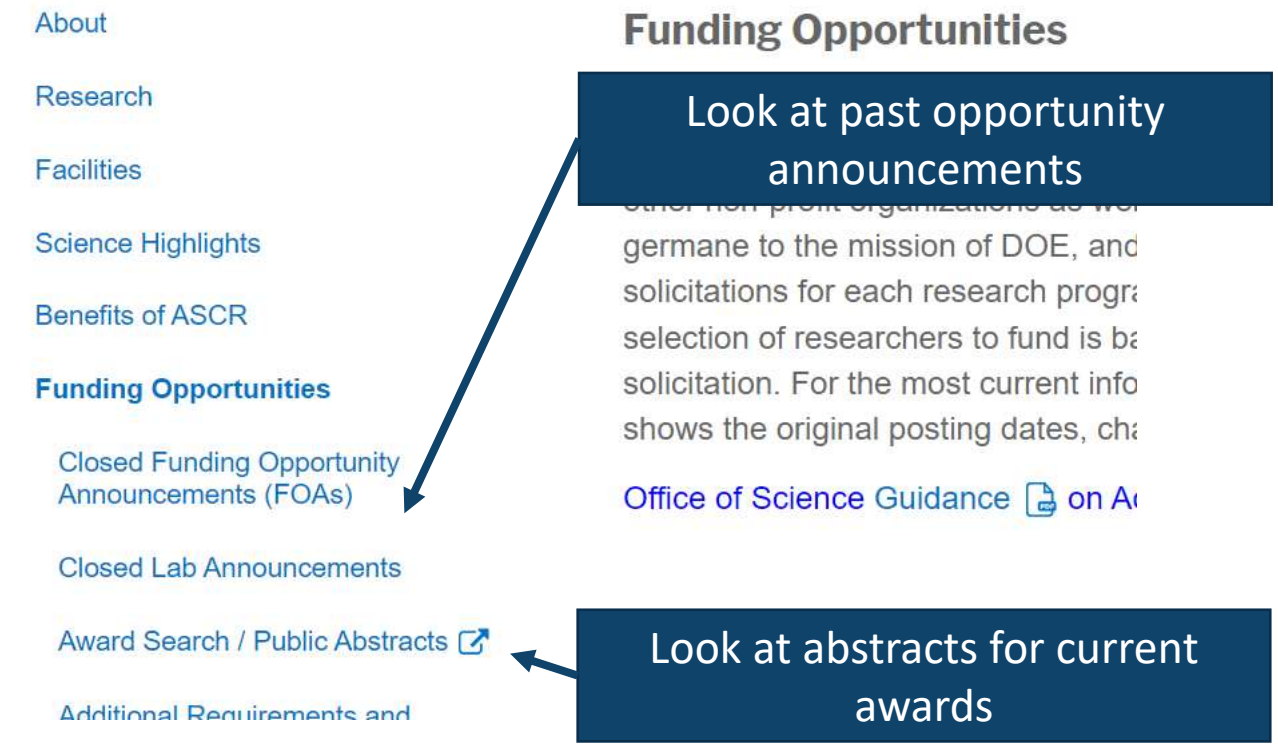


Slice through combined HACC/Nyx simulation

Additional Information on ASCR's Website

https://science.osti.gov/ascr/Funding-Opportunities

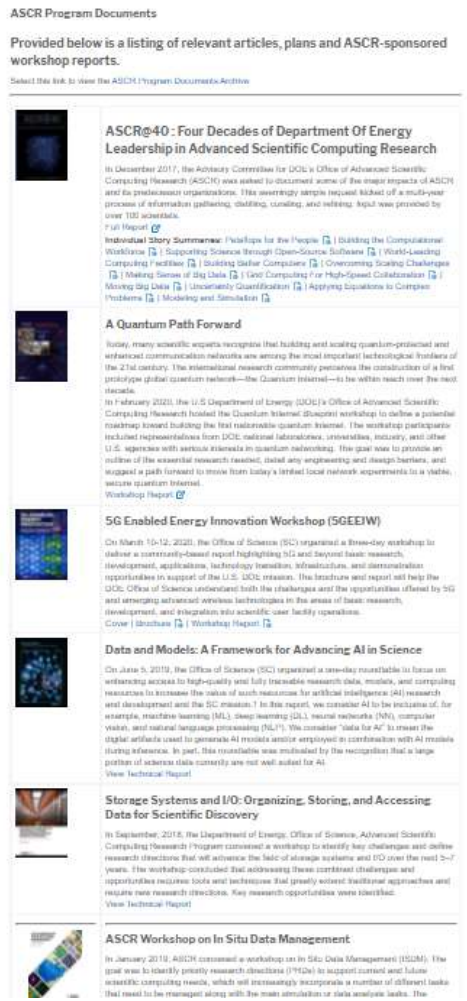
https://science.osti.gov/ascr/Community-Resources/Program-Documents



Look at past opportunity announcements

Look at abstracts for current awards

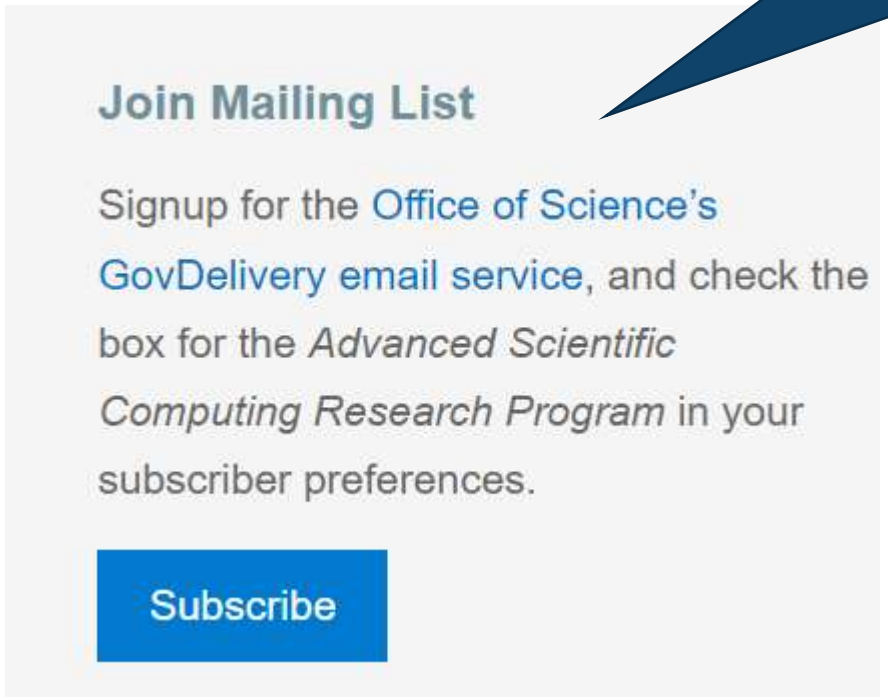
Look at recent reports from ASCR-sponsored workshops. These discuss priority research directions, as identified by the research community, along with relevant background information, in various areas.



Finding Out More About ASCR – GovDelivery

For updates from ASCR (announcements for ASCAC meetings, FOAs, awards, workshops, etc.) signup for the GovDelivery email service.

This link is near the bottom of https://science.osti.gov/ascr



The DOE SciDAC Team

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  - **Steven Lee** (ASCR/FASTMath)
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- **ASCR SciDAC Partnerships**
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  - **Marco Fornari** (ASCR/BES)
  - **David Rabson** (ASCR/NE and OE)
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