LLNL FESP Theory Highlights: November 2024

Editor: Ben Dudson (Group Leader), on behalf of the LLNL Fusion Theory & Modeling group.

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Contents

Invited presentations

M. Sengupta and M. D. Campanell, "Sheath transitions in the two-plasma mode of a filament discharge-- Aid-Compete Effects", Invited Talk at the 8th Asia-Pacific Conference on Plasma Physics (AAPPS-DPP 2024) in Malacca, Malaysia. Presented on November 4th 2024.

This talk presented a refined understanding of plasma-facing thermionic emitter cathodes by examining the limitations of the conventional space charge-limited model, which overlooks ion trapping dynamics within the virtual cathode. While conventional theory distinguishes between temperature-limited and space charge-limited regimes based on electron current constraints, recent findings reveal that trapped ions can form a quasi-neutral "second plasma," expanding upstream and interacting with the primary plasma. These effects are amplified in non-planar geometries, such as cylindrical or spherical sheaths, where trapped ions create a positive feedback loop with the upstream plasma. To address these phenomena, a new "Aid-and-Compete" model was developed, offering insights into current enhancement and sheath mode transitions relevant for plasma devices, including emissive cathodes in electric propulsion, fusion applications, thin film deposition systems, and plasma diagnostics.

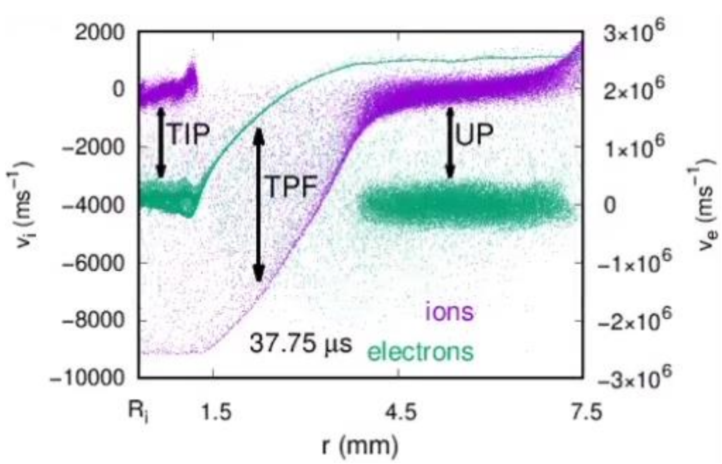


Fig. 1 (left): The two-plasma mode in a cylindrical coaxial discharge. Scatter plots of electrons and ions in radial phase space illustrate: (1) a Trapped-Ions Plasma (TIP) near the inner cathode filament (left); (2) an accelerating Double Layer with Transported Particle Fluxes (TPF) at intermediate radii; and (3) an Upstream Plasma (UP) at larger radii (right). The outer anode shell is located at a radius of 7.5 mm.

Ben Zhu, **Menglong Zhao**, **Xue-qiao Xu**, Harsh Bhatia, Peer-Timo Bremer, **Thomas Rognlien**, **William Meyer**, Anchal Gupta, KyuBeen Kwon, Xinxing Ma, David Eldon, Hyungho Lee, and Junghoo Hwang, "Latent Space Mapping: Revolutionizing Predictive Models for Divertor Plasma Detachment Control", invited talk, 66th Annual Meeting of the APS Division of Plasma Physics (APS-DPP), Atlanta, GA, October 11, 2024

The invited talk presents the LLNL and its collaborators' effort on the development and application of surrogate models for controlling plasma detachment in magnetic confinement fusion (MCF) devices, a critical aspect of managing heat and particle exhaust in future fusion reactors. Due to the loss of critical in-situ diagnostics and long latency in future reactors, the new detachment control needs fast and reliable boundary and divertor plasma models. The data-driven surrogate model approach addresses these challenges by providing a quasi-real-time solution that can predict divertor conditions without running time-consuming simulations. The latest surrogate model, based on approximately 70,000 2D UEDGE simulations of KSTAR tokamak, uses a two-stage training process involving an auto-encoder for dimensionality reduction and a multi-layer perceptron for self-consistent prediction of both upstream and downstream plasma conditions, is capable of making predictions in less than 0.1 milliseconds with a relative error of less than 25% compared to UEDGE simulations. With the demonstration of quasi-real-time prediction capability, which is crucial for operational control in fusion reactors, Model Predictive Controls (MPCs) are being developed to manage actuator latency in future large machines (see Figure 1). A prototype of such a control is set to be tested as an observer in the upcoming KSTAR campaign. In the meantime, ongoing work includes further improving the surrogate model and exploring other applications in magnetic fusion energy (MFE) research and development.

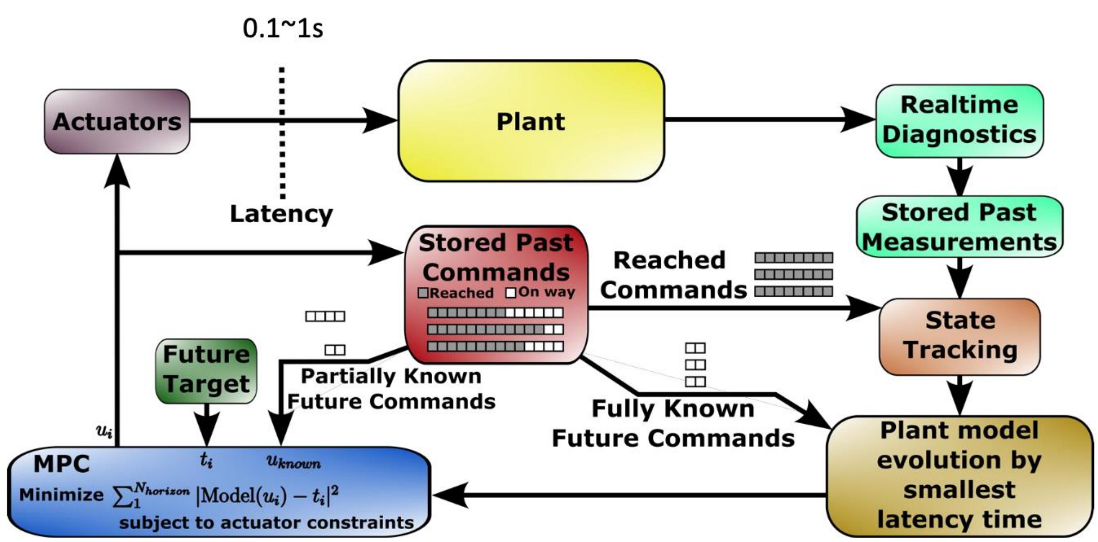


Fig. 2 (above). Sketch of a possible Model Predictive Control (MPC) for high latency system control. Here our surrogate model can be used in "State tracking", "Plant model evolution", and "MPC".

Conference presentations and posters

M. Zhao, **B. Zhu**, **T. Rognlien**, **X. Xu**, W.H. Meyer, K. Kwon, X. Ma, D. Eldon, **N. Li**, H. Lee, J. Hwang, *UEDGE database for KSTAR detachment control*, oral presentation at 66th APS-DPP, October 7, 2024, Atlanta GA.

We built a database of ~78000 2D UEDGE runs with cross-field drifts, by varying 5 control parameters: input power, core boundary density, particle and thermal diffusivity, impurity fraction and plasma current, for developing surrogate models (see Ben Zhu's highlights) to improve the control algorithm for KSTAR detachment control.

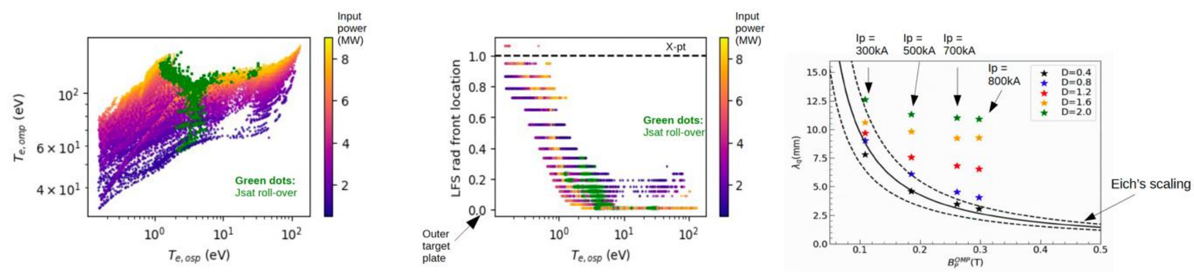


Fig. 3 (above). **Left**: Outer mid-plane electron temperature Te,omp as a function of outer strike point temperature Te,osp for various input power, diffusivities and impurity fractions. Outer target detachment onset (Jsat roll-over) occurs when Te,osp ~ 3 eV; **Middle**: Location of the low-field side radiation front as a function of Te,osp. The LFS radiation front is about to move away from the plate when detachment onset occurs.

I. Novikau, **I. Joseph**, Quantum algorithm for solving nonunitary truncated Koopman – von Neumann equation, talk, SQuInt 2024 Annual Workshop, October 30 – November 1, Boulder, CO

Quantum computers (QCs) have the potential to speed up simulations of plasma dynamics, which requires dealing with large amounts of high-dimensional data, by leveraging superposition and entanglement. We have developed block-encoding techniques that enable quantum simulation of linear fluid and kinetic plasma wave dynamics using the well-known QSP and QSVT algorithms.

Due to the no-cloning theorem, nonlinear (NL) dynamics is challenging for QCs. The Koopman-von Neumann (KvN) approach overcomes this issue by embedding the system into a linear advection equation for the probability distribution function. Unitary discretizations for the advection operator tend to lead to unphysical numerical oscillations. Hence, we use an upwind discretization to add dissipation and turn the KvN model into an advection-diffusion equation. We use the Linear Combination of Hamiltonian Simulations algorithm to provide an explicit encoding of the dissipative dynamics in terms of multiple unitary evolution operators. Combining the LCHS and KvN techniques leads to a new quantum algorithm (QA) for simulating NL dynamics. We provide an explicit block encoding of a NL test problem and simulate the LCHS-KvN quantum circuit on a digital emulator of fault-tolerant quantum computers. We analyze the circuit's scaling and success probability and discuss the range of possible applications.

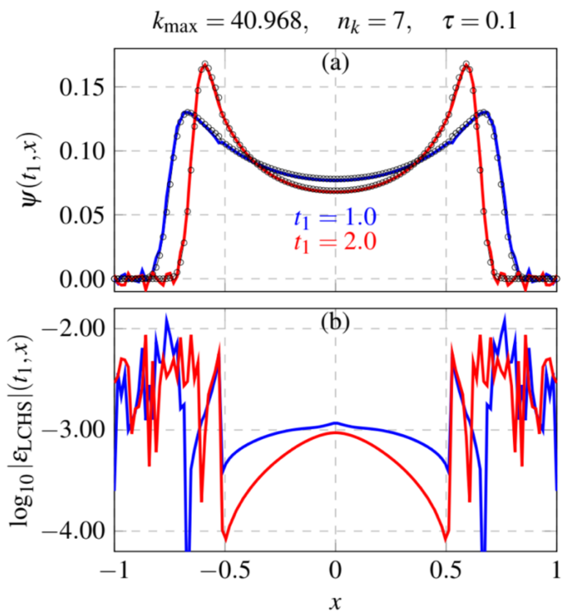


Fig. 4 (left): Results from simulations of the truncated KvN embedding technique for a nonlinear problem with two fixed points. **(a)**: Classical simulations (black markers) and simulations of the LCHS-KvN circuit on a digital emulator of fault-tolerant quantum computers (colored solid lines). **(b)**: The corresponding errors of the LCHS-KvN simulations.

M. D. Campanell, "Mechanisms limiting the electron current from a surface through a plasma", presented as a poster at the 77th Annual Gaseous Electronics Conference in San Diego, California, October 1, 2024.

This presentation demonstrated that the current of emitted electrons from a cathode through a plasma can be limited not only by the conventional "space charge effect" but also by a second mechanism termed "backflow saturation". Depending on conditions, backflow can set a much lower limit on the transmittable current than space charge. Backflow saturation also results in unconventional potential distributions and sheath voltages throughout the electrode gap. The backflow effect is predicted to play a role in plasma physics research areas where surface-emitted electron currents are important. Examples include low temperature plasma technologies with thermionic cathodes, and possibly ITER divertors with strong thermionic emission from tungsten targets.

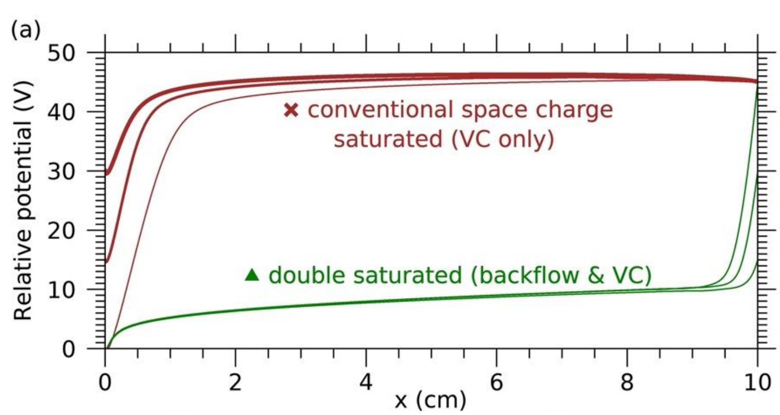
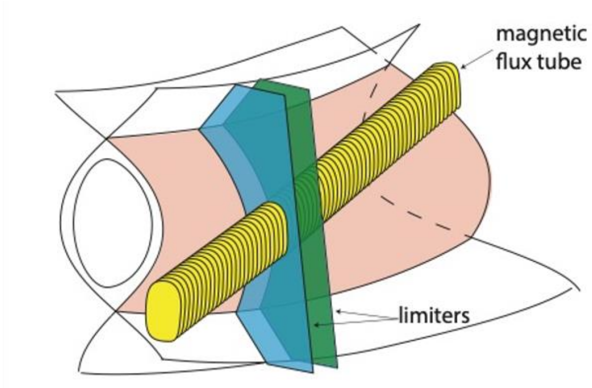


Fig. 5 (above). Comparison of potential distributions between a thermionic cathode and anode under two forms of current limitation. The conventional picture of space charge saturation accounts for only a virtual cathode (VC). The newly demonstrated scenario includes backflow saturation where the cathode sheath collapses to such a weak voltage that electrons from the interior plasma can return to the cathode, thereby reducing the overall current reaching the anode.

M.V. Umansky, "Hermes simulations of RF antenna in tokamak edge plasma show induced convective cells and turbulent transport." Talk presented at the RF SciDAC team meeting.

In the RF SciDAC we are modeling the impact of an RF antenna on plasma and impurity transport, using 3D flux-driven turbulence simulations in a flux tube partially intercepted by biased limiters. These 3D simulations are performed with the drift-fluid Hermes-3 code built on BOUT++, that was developed under the Theory & Computations base theory program.



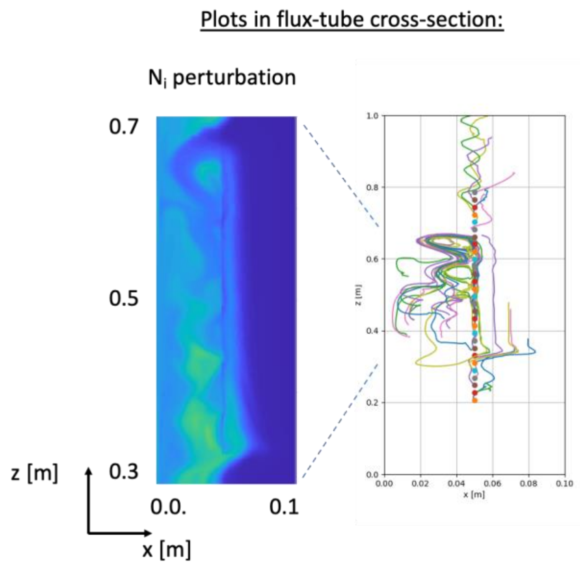


Fig. 6 (above): The simulation geometry is a flux tube in the Scrape-Off Layer (yellow). The flux tube intersects limiters representing the RF antenna (blue & green). It terminates at the upper and lower divertor targets.

(right): Plasma fluctuations and profiles are modified by the mean RF antenna bias. Impurity ion tracing reveals enhanced transport

Radio Frequency (RF) antennae in contact with plasma create significant bias voltage, due to the asymmetric response of plasma sheath current to oscillating electric fields. The RF oscillation frequency is much higher than the plasma dynamics so is not included in the simulation, but the resulting bias voltage leads to plasma flows. Hermes-3 simulations show the emergence of convective cells that modify turbulent plasma profiles (shown in Fig. 6 right). Using passive tracers in the resulting ExB flows, we find that the turbulent transport level is comparable to experiment, and that the RF bias voltage enhances transport of impurities from the antenna housing into the plasma. These novel results are now being developed into a publication.

Y. Fu, B. D. Dudson, X. Chen, M. V. Umansky, F. Scotti, T. D. Rognlien, "Statistical inference of anomalous thermal transport with uncertainty quantification in the plasma boundary" Poster presentation at 66th Annual Meeting of the APS Division of Plasma Physics (APS-DPP), Atlanta, GA, October 10, 2024

In this presentation, the critical task of inferring anomalous cross-field transport coefficients is addressed in fluid-based plasma boundary simulations essential for optimal design of tokamak divertors. We developed an integrated workflow of parameter inference in the UEDGE fluid code using Bayesian Optimization (BO), which is a global optimization method suitable for optimization of computationally expensive objective functions. In the workflow, transport coefficients are inferred by minimizing a user-defined loss function, such as the discrepancy between UEDGE profile and observations. Uncertainty Quantification (UQ) is also integrated throughout the optimization to enable the efficient evaluation of the tokamak component design against plasma performance.

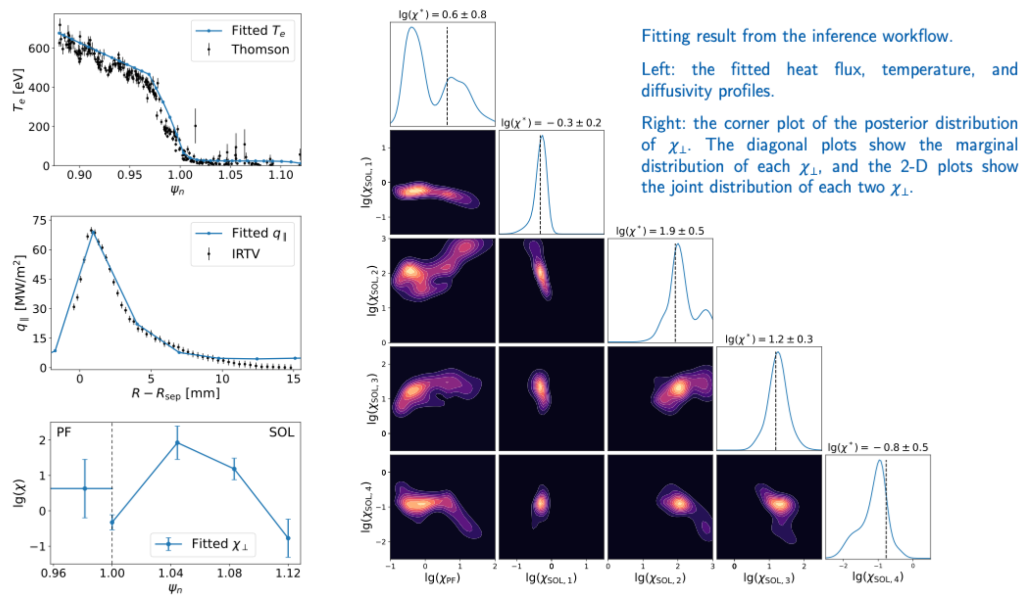


Fig 7 (above): Inference of UEDGE transport parameters from experimental data.
The Bayesian Optimization workflow identifies optimal parameters and their posterior distribution.

Y. Fu, H. Qin, “Topological waves in cold and MHD plasmas: a perspective of spectral flow”. Contribution talk at 66th Annual Meeting of the APS Division of Plasma Physics (APS-DPP), Atlanta, GA, October 9, 2024.

This talk summarized Y. Fu’s thesis work, which discussed the recent study of the topological properties of linear plasma waves. We presented a rigorous description of the wave topology based on the spectral flow theorem. A topological mode in continuous media is understood as the spectral flow induced by the nontrivial topology of the eigenmode bundle over a sphere surrounding the phase-space Weyl point. We discussed two examples of the topological waves in cold and Hall MHD plasmas from the perspective of spectral flow. The cold plasma model is Hermitian and supports the topological Langmuir-cyclotron waves. The Hall MHD model is non-Hermitian but PT-symmetric, supporting the topological Alfvén sound wave.

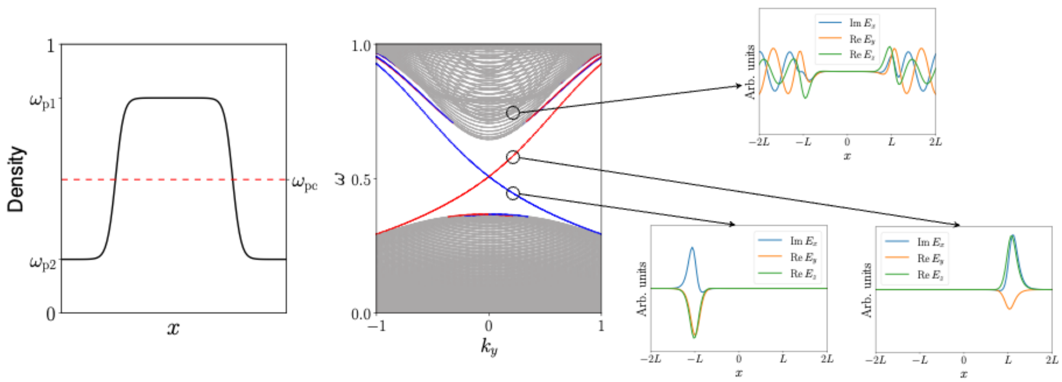


Fig. 8 (above): A demonstration of topological surface waves in cold magnetized plasmas. The plasma density is shown in left, the dispersion relation is shown in middle. Gray curves represent “bulk” waves, whose eigenfunctions are plane waves; the blue and red curves are “topological surface” waves, whose eigenfunction localized near the density gradient.

Publications

Yichen Fu, Justin R Angus, Hong Qin**, Vasily I Geyko**, “Exactly energy-momentum-conserving stochastic differential equations and algorithms for nonlinear Landau-Fokker-Planck equation”, arXiv preprint, arXiv:2410.12079.

This paper discussed a new set of stochastic differential equations (SDE) for Columb collisions described the nonlinear Landau-Fokker-Planck equation. The new set of SDE conserves energy and momentum exactly, which is lacking in tradition SDEs for Columb collisions. Therefore, those new SDE presents new understanding of the governing microscopic stochastic process of Columb collision. An exactly conservative numerical algorithm was also developed and benchmarked with analytical theory.

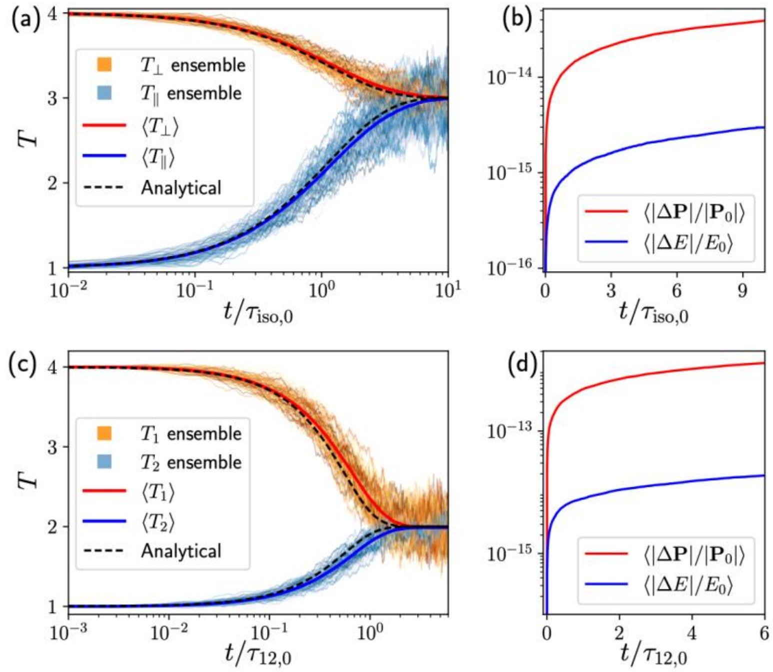


Fig 9 (above): Benchmark of SDE with analytical theory for two relaxation processes. (a), (b): intra-species temperature isotropization. (c), (d): inter-species temperature relaxation. (a), (c): the first 100 sample patches are shown with a color gradient, and the average temperature and analytical solution are shown in solid and dashed lines. (b), (d) are average absolute errors in energy and momentum

International visitors

November 11 – 14, 2024: UK's Hartree Center visits LLNL

Researchers from the United Kingdom's Hartree Center visited LLNL to continue discussions of collaborations in advanced algorithms and Machine Learning for fusion energy.

DOE SC Artificial Intelligence (AI) Initiative Roundtables

October and November, 2024

Ben Zhu, representing FES researcher at LLNL, attended the SC AI roundtable on Fabrication Science as an observer from October 30-31, 2024. In addition, LLNL's MCF ML/AI-related work (e.g., ML model of advanced fluid closure, interference of missing measurement based on partial observations, data-driven surrogate model of boundary plasma) are summarized and presented at the SC AI roundtable on Fundamental Energy Research from November 6-7.