2023 INCITE Proposal Submission
Proposal

Title: Hybrid simulation of macroscopic instabilities with energetic particles in fusion plasma

Principal Investigator: Chang Liu

Organization: Princeton Plasma Physics Laboratory

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Section 1: PI and Co-PI Information

Question #1

Principal Investigator: *The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

Principal Investigator

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Question #2

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Last Name

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Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

Institutional Contact Name

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Physics: Plasma Physics

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

We will use the M3D-C1-K code to conduct kinetic-MHD simulation for magnetohydrodynamics (MHD) instabilities excited by energetic ions or runaway electrons in tokamaks and stellarators. The goal is to understand the comprehensive nonlinear physics in current experiments and solve critical physics issues for ITER and future magnetic confinement fusion reactors.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an Early Career Track in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

***Who Can Apply**: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would*

you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.

- *What review criteria will be used for the Early Career Track?*
  - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

Yes

If 'yes', what year was your PhD? If 'no' enter N/A

2017

If 'yes', how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

I (Chang Liu) am currently a staff research physicist at Princeton Plasma Physics Laboratory. I did my PhD at PPPL doing research on runaway electron physics in tokamaks. I joined the M3D-C1 code group in 2019 and the focus of my research is to develop a kinetic-MHD framework based on the MHD simulation code M3D-C1 and optimize it for GPUs. In the past 3 years I have finished developing the kinetic module of M3D-C1 (M3D-C1-K) and did the GPU optimization for particle-pushing and MHD calculation, and used the developed code to study linear and nonlinear physics of energetic particles. In addition, using the knowledge from my previous work, I developed a runaway electron simulation module in collaboration with others, and published papers on nonlinear simulation of MHD modes in DIII-D tokamak disruptions in presence of runaway electrons.

Currently I receive funding support from 3 SciDAC centers, ISEP, SCREAM and CTTS. For ISEP the focus of research is MHD instabilities driven by energetic ions (Alfvén modes, fishbone modes, etc). For SCREAM and CTTS, the focus is runaway electrons including their coupling with MHD instabilities and finding mitigation strategy for high-energy runway electron beams. I will also do simulation work supporting research on NSTX tokamaks, where phenomena like fishbones and Alfvén mode avalanches have been frequently observed. The simulation runs proposed in this INCITE project are closely related to my research in the next 5 years, and I believe that the computational resources can enable us to do unprecedented research to explain the mysteries in tokamak and stellarator experiments and expand the frontier of our knowledge on energetic particle physics. It is also important for us to achieve the milestones of the SciDACs. In addition, I am participating the Joint Institute for Fusion Theory (JIFT) program which involves exchange of scientists between US and Japan on fusion research. I will use this chance to collaborate with Japanese physicists and computationists including code benchmarks and improving our knowledge on code optimization on different computer architectures.

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Node Hours

240,000

Storage (TB)

120

Off-Line Storage (TB)

100

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

1,000

Storage (TB)

10

Off-Line Storage (TB)

10

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Node Hours

240,000

Storage (TB)

120

Off-Line Storage (TB)

120

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel Xe) Resource Request – 2023

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Funding Source

US Department of Energy

Grant Number

DE-SC0016268

Funding Source

US Department of Energy

Grant Number

DE-SC0018109

Funding Source

US Department of Energy

Grant Number

DE-AC02-09CH11466

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Section 5: Project Narrative and Supplemental Materials

Question #1

Using the templates provided here, please follow the INCITE Proposal Preparation Instructions to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

2023_INCITE_New_Project_ChangLiu.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title (*80 characters max; strictly enforced*): Hybrid simulation of macroscopic instabilities with energetic particles in fusion plasmas

PI and Co-PI(s): Chang Liu, Stephen Jardin, Amitava Bhattacharjee

Applying Institution/Organization: Princeton Plasma Physics Laboratory

Number of Processor Hours Requested: 240,000 node hours on Summit (Year 1), 240,000 node hours on Frontier (Year 2)

Amount of Storage Requested: 120 TB on Summit (Year 1), 120 TB on Frontier (Year 2),

Executive Summary *(May use the remainder of page)*:

The interaction of high energy particles such as energetic ions and runaway electrons with the mascroptic instabilities happening in plasma plays a critical role in the performance of magnetic confined fusion reactors like tokamaks and stellarators. Alfvén modes can be driven unstable by energetic ions and lead to energy deconfinement. The runaway electrons can alter the properties of magnetohydrodynamic instabilities happening in a tokamak disruption, and uncontrolled high-energy runaway electron beams can cause severe damage to the device. The nonlinear behavior of macroscopic instabilities associated with energetic particles can only be simulated using high-performance computers due to the wide range of timescales.

In this proposal, we plan to use the kinetic-MHD code M3D-C1-K to simulate macroscopic instabilities in the presence of energetic ions or runaway electrons. The objective is to better understand the comprehensive physics of the interactions, to explain phenomena observed in current fusion experiments, and to make predictions for future reactors like ITER. The research work is supported by three SciDAC centers, ISEP, SCREAM and CTTS. The M3D-C1-K code was developed based on a mature implicit high-order finite-element MHD code M3D-C1. Key components of the code have been optimized for GPU and impressive speedup compared to the CPU version has been achieved. For energetic ions, we plan to conduct nonlinear simulation using a 3D mesh to study the wave-particle interaction between the energetic ions and Alfvén modes, including mode-mode coupling effects. We plan to study the frequency chirping of modes and zonal flow generation, and to do long time simulations involving simultaneous excitation of multiple modes and abrupt large-amplitude events, which have been observed in DIII-D and NSTX experiments. For runaway electrons, we plan to simulate MHD instabilities happening during disruptions in tokamaks in the presence of strong runaway electron generation. The goal is to model the loss of runaway electrons during the breakup of magnetic flux surfaces and find the best strategy to minimize their destructive effects.

In summary, we believe that the project will target some of the most important issues in the field of magnetic confined plasma physics which are critical to the success of fusion energy. The numerical simulations in this project will have a high impact and will inspire future theoretical, numerical, and possibly experimental work.

PROJECT NARRATIVE

SIGNIFICANCE OF RESEARCH

Fusion power is often regarded as the most promising clean energy source with several advantages over fission power. The concept of magnetic confinement fusion, including tokamaks and stellarators, is being studied in laboratories around the world. The International Tokamak Experimental Reactor (ITER), the world's largest international collaborative experimental project, is due to produce its first experimental plasmas in 2025. In addition to experiments, numerical simulation codes have been developed to model the physics behavior of the plasma confined in the device,in order to optimize the performance and avoid disruptive events. To progress from laboratory experiments to a commercially viable fusion reactor, several challenges need to be overcome. Two of them are the confinement of energetic particles (EPs) and the control of high-energy runaway electrons (REs). In this project we plan to use the M3D-C1-K code to address these physics issues, paving the way for the success of ITER and future fusion reactors.

Energetic ion physics

Energetic ions are ubiquitous in plasmas in magnetically confined fusion devices. They can be produced as the result of fusion reactions (alpha particles) or from neutral beam injection (NBI) or other non-inductive heating. Their energy can range from hundreds of keV to several MeV, which is much higher than the thermal temperature of the bulk plasma. In order to achieve self-sustained nuclear fusion reaction, or "ignition", self-heating from EPs is necessary to compensate for energy loss due to transport. Therefore, adequate confinement of energetic ions is essential for the success of fusion reactors [1].

It is well known that macroscopic instabilities can cause transport of energetic ions due to resonant interactions between waves and particles [2]. These instabilities include high frequency magnetic oscillations, or Alfvén waves, and low frequency modes like "fishbone" modes. The instabilities can be driven by energetic ions themselves due to their free energy and spatial gradient. These modes have been observed in most magnetic fusion experiments, and are predicted to play an important role in ITER.

In previous work, various kinds of macroscopic instabilities driven by energetic ions have been studied, including their dispersion relations and excitation mechanisms. A large portion of these studies focus on the linear property of the modes, which is only valid when the mode has small amplitude at the early stage of their excitation. The study of the nonlinear behavior of these macroscopic modes can only be done through long-time numerical simulations as there is a large time scale separation between the wave period and the nonlinear evolution timescale. Various nonlinear physics associated with Alfvén modes excited by energetic ions have been discovered in experiments, including frequency chirping of the Alfvén waves after saturation, the intermittency behavior of mode excitation and saturation, and the generation of zonal flows as a result of mode-mode coupling. Interestingly, the zonal flows generated from Alfvén modes can suppress further growth and reduce the transport of the energetic ions. In ITER, it is likely that multiple Alfvén modes can be excited simultaneously which can lead to abrupt large-amplitude events (ALE) with nonlinear effects becoming more important.

Runaway electron physics

Runaway electrons are high-energy electrons accelerated by the inductive electric field as a result of disruption, which is a kind of event that terminates the normal operation of a tokamak. In a disruption, the energy confinement of the plasma is suddenly lost due to macroscopic instabilities, and the plasma temperature can drop from keV to a few eVs. On the other hand, runaway electrons can gain energy from this event to MeV range, and their population can increase exponentially due to an avalanche process. If not well-controlled, runaway electron beams can cause severe damage to vessel walls and result in

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months of repair time. This can become a serious problem for ITER and future fusion reactors based on tokamaks, therefore the studies on disruption avoidance and runaway electron mitigation has become priority for ITER research [3].

Simulating runaway electrons is a challenging job even for high-performance computing (HPC). The relativistic runaway electron beam can stream along the magnetic field lines inside a fusion device with velocity close to the speed of light, but their interaction with the plasma can occur over timescales of microseconds or even milliseconds. This large time scale separation means that classical particle simulation methods may not be practical. To test the various strategies of runaway electron mitigation, an integrated simulation model including comprehensive physics is required. The relevant physics includes MHD instabilities like kink modes and vertical displacement events (VDE), pellet injection, and resonant magnetic perturbations (RMPs). In addition, in order to do validation studies and compare with experimental results, synthetic diagnostic tools such as radiation power and spectrum calculation also need to be developed.

Kinetic-MHD model

Traditionally, the macroscopic instabilities in plasma can be simulated by solving the magnetohydrodynamics (MHD) equations, which calculate the evolution of the first few moments of the particle distribution, assuming they follow a Maxwellian distribution. Similar to a fluid simulation, the method reduces the dimensions of the problem and introduces closures for high-order effects. However, both energetic ions and runaway electrons can be regarded as outliers of the bulk particle population, or the high-energy tail beyond the Maxwellian distribution. Even though their population is much smaller compared to thermal ions and electrons, they can play important roles in affecting the MHD instabilities in plasmas. These energetic particles can provide the free energy to drive the MHD modes unstable. Note that both energetic ions and runaway electrons have distributions in velocity space that are different from Maxwellian, thus their collective behavior may not be accurately described using a fluid model. In addition, these particles can have more chances to resonate with the waves, which can only be studied by taking a kinetic approach.

In order to simulate macroscopic instabilities driven by energetic particles, two approaches can be taken. The first one is fully kinetic simulation, in which both energetic particles and thermal particles are simulated using a kinetic method. In this approach, the simulation domain is extended to include the velocity space of all particles, either through a continuum description or using the particle-in-cell (PIC) method. Although this approach incorporates all the necessary physics and gives the most complete picture of the instabilities, the computation can be very expensive as a large number of grids or markers are required to simulate the tremendous amount of particles, to avoid numerical noise and error accumulation. The second approach is the kinetic-MHD simulation, which is a hybrid approach trying to bridge the classical MHD model and the kinetic method. In this model, the thermal ions and electrons are still described using the MHD equations, while the energetic particles are modeled using the PIC method. The two models are then coupled together through “pressure-coupling” or “current coupling”. In this model, the PIC simulation provides closures for the MHD simulation which provides additional information regarding the kinetic effects of energetic particles that can affect the macroscopic instabilities. Since the energetic particles are only minority species compared to the thermal particles, the cost of simulating them using PIC is much less compared to the full-kinetic approach, and the key physics such as wave-particle interaction for the energetic particles are still kept.

Introduction to M3D-C1-K code

Several simulation codes have been developed based on the kinetic-MHD simulation model, including M3D-K [4], NIMROD [5], XTOR-K [6], MEGA [7] and CLT-K [8]. MEGA was originally

developed at National Institute of Fusion Science (NIFS) in Japan, and is now widely used to model energetic ion driven MHD instabilities in stellarators and tokamaks around the world. The code utilizes explicit methods to calculate the particle motion and the evolution of the MHD equations, and can handle complicated 3D geometry. The MEGA code has been used for long-time nonlinear simulation for ALE in JT-60 tokamak using Japanese supercomputer JFRS-1 [9]. A similar code, CLT-K, is now being actively developed in China. Most of the existing kinetic-MHD codes have not been optimized for GPUs, meaning that they cannot utilize the current-gen and next-gen supercomputers in the United States like Summit and Frontier.

M3D-C1-K is a new kinetic-MHD code which is developed on the basis of a mature finite element MHD code M3D-C1 developed by Stephen Jardin and Nathaial Ferraro at Princeton Plasma Physics Laboratory. The M3D-C1 code can solve MHD equations in an unstructured mesh using a high order finite element [10]. Thanks to the advanced semi-implicit method, the code can advance the equations with a large timestep and avoid numerical instabilities, thus is suitable to simulate plasma instabilities and nonlinear evolution happening in a long timescale. The "K" stands for kinetic, which can be used to simulate energetic ions and runaway electron physics using PIC and delta-f methods. In addition to tokamaks, the code has recently been extended to simulate MHD instabilities in stellarators [11].

We have taken efforts to optimize different parts of the code for GPUs. Through participating in the GPU Hackathon at Princeton University in 2019, we developed a new version of the particle pushing code in the kinetic module for energetic ions, and reached about 30 times speedup compared to the old version running on CPUs. Encouraged by this progress, we have tried to use a similar technique to optimize the runaway electron simulation model in the code, and got a similar speedup. Both the energetic ion and runaway electron GPU code have been tested on Summit, though the Director's Discretion (DD) project at OLCF we applied in 2020. In addition, we recently tried to port the calculation and assembling of the finite element matrix for the MHD equations to GPUs, through the participation of another GPU Hackathon in 2021. The porting was successful and we reached another 20 times speedup for the matrix calculation part. The work has been selected as an invited talk in the 2022 OpenACC Summit. The assembled matrix is then solved using the PETSC library. This part of the code is still running on CPU now, but there is an ongoing effort from the Lawrence Berkeley National Lab (LBL) for optimizing the SuperLU solver on GPUs. They have reached about 2-5 times speedup on a single GPU, and the capability of utilizing multiple GPUs will be included in the next release.

Several scientific results have been published with the help of M3D-C1-K. We have used the code to do linear and nonlinear simulation of fishbone modes [12] and Alfvén modes [13] driven by energetic ions using parameters from tokamak experimental devices like DIII-D at Generation Atomics and National Spherical Torus Experiment (NSTX) at the Princeton Plasma Physics Laboratory (PPPL), and compared the results with other established codes. In addition, we have successfully done a nonlinear simulation for MHD instabilities happening in a tokamak disruption event with a significant amount of runaway electrons, and obtained good agreement with the DIII-D tokamak experiment [14]. New results of integrated simulation including a self-consistent source term for runaway electron generation and their interaction with injected pellets are now in preparation for publication. These works are supported by three Scientific Discovery through Advanced Computing (SciDAC) centers, the Integrated Simulation of Energetic Particles in Burning Plasmas (ISEP), the Simulation Center for Runaway Electron Avoidance and Mitigation (SCREAM), and Center for Tokamak Transient Simulation (CTTS).

In summary, we believe that the work proposed here can be impactful to the fields of energetic ions and runaway electrons physics. Although we have done linear and quasilinear simulations before to address several issues, the more complicated problems, like the intermittency behavior and mode-mode coupling in ALE, can only be simulated using large-scale supercomputers like Summit or Frontier. This can be an important step towards whole-device modeling of tokamaks and stellarators, and can help build

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a reliable predictive tool for the basis of the development of reduced models or data-driven machine learning studies. We also plan to use the allocated resources to do tokamak disruption simulations, to better understand runaway electron physics and find the best mitigation strategy, which can be an important matter for the success of ITER. By doing verification and validation work with other codes like MEGA, we can further improve the physics model in M3D-C1-K. With the help of computational resources from OLCF, we expect that we can do long-time nonlinear simulation of kinetic-MHD to address critical physics issues and explore the frontier of plasma physics.

RESEARCH OBJECTIVES AND MILESTONES

In this 2-year project, we plan to study the MHD instabilities excited by energetic ions in the first year, and do integrated simulations of tokamak disruption with runaway electron and MHD instabilities in the second year. For energetic ions, we will focus on the physics of Alfvén mode frequency chirping and zonal flow generation, and do long-time ALE simulation including the nonlinear interaction between multiple excited Alfvén modes. For the runaway electron physics, we will start with discrete physics issues including high-frequency current-quench modes and low-frequency MHD modes excited by runaway electrons, and then do integrated simulations of tokamak disruption including runaway electron generation and pellet injections.

Research Objectives of Energetic Ion studies

Understand Alfvén mode frequency chirping

Rapid frequency chirping of Alfvén modes have been observed in tokamak and stellarator experiments. The chirping is often associated with the formation of holes and clumps in particle phase space, due to the dissipative effects like resistivity and viscosity, and the collective movement of resonant particles [15]. There has been a theoretical calculation of chirping rate for the marginal cases, when the mode drive is slightly larger than the damping, and the mode is just above its excitation threshold. Nonlinear simulation of the chirping of a single mode has been done with other kinetic-MHD codes like MEGA [7] and CLT-K [8], and has also been done with reduced simulation models. The simulation results show good agreements with the theory in certain cases, but also show disagreements when the mode is far away from the stability boundary. In addition, it is found in the simulations that the mode can have cyclic “rebirth” at the original frequency when the initial mode branch has chirped to a different frequency. In addition to fusion devices, the frequency chirping of Alfvén and whistler modes has also been observed in space plasma like the magnetosphere of the earth [16].

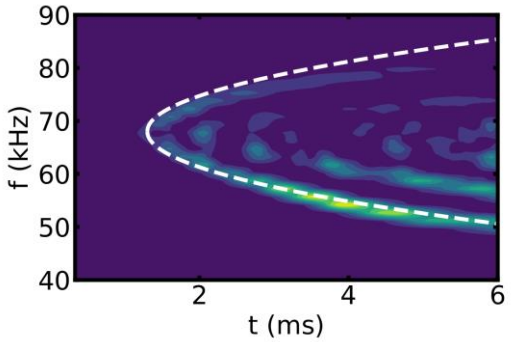

Fig. 1. Spectrogram of simulation results using M3D-C1-K of RSAE chirping in DIII-D, compared with theoretical results (white dashed lines).

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We have done nonlinear simulation of M3D-C1-K to study the chirping of a single reversed-sheared Alfvén eigenmode (RSAE) in DIII-D. The initial result shows reasonable agreement with the theory regarding the chirping rate (Fig. 1), and we capture the movements of resonant particles in phase space. For the INCITE project, we plan to extend the simulation to include multiple modes and study the behavior of chirped mode in the longer timescale. We will also study the detailed dynamics of resonant particles in phase space, including the resonance broadening effects and overlapping of multiple resonance regions, in order to gain better understanding of the chirping mechanism and build a better theoretical model. We will also use the nonlinear simulation to study the evolution of MHD mode structure during the frequency chirping, and compare with the experimental observations. For the long-term goal, we plan to study the frequency chirping of other modes such as compressional Alfvén eigenmodes (CAEs) and whistler modes, which have higher frequency than the RSAEs and thus require more computational resources.

Nonlinearity of Alfvén mode and zonal flow generation

When the Alfvén mode is strongly excited by energetic ions, it can deviate from its linear dispersion relation and the high-order terms associated with interaction with itself or with other modes become more important. In previous studies of the nonlinear evolution of low wavenumber modes, the self-interaction was found to be important, which can drive flow structure with zero wavenumber in the toroidal and poloidal directions (k_φ=k_θ=0), or zonal flows. The nonlinear interaction can have complicated effects on the plasma and energetic ion confinement. On one hand, the overlapping modes can break the nested flux surfaces and lead to formation of stochastic fields in the tokamak, which can significantly enhance the particle transport. On the other hand, the generated zonal flows can suppress the turbulence and the associated anomalous transport, therefore improving energy confinement. The latter effect has been observed in the Joint European Torus (JET) experiment recently and attracted a lot of attention. In order to better understand this complicated phenomena, nonlinear simulation with control variables are necessary.

In this project we plan to continue the simulation of zonal flow generation in the nonlinear simulation of a single mode, and understand the dependence of generated flow on plasma parameters. In our previous simulations, it has been found that the generated zonal flow can suppress the growth of the Alfvén mode and lead to a fast decay of it (Fig. 2). We will also perform simulations to study the interaction of multiple modes, which can excite not only zonal flows but also modes with nonzero wavenumbers, to have a more complete and realistic picture of mode interaction in tokamaks.

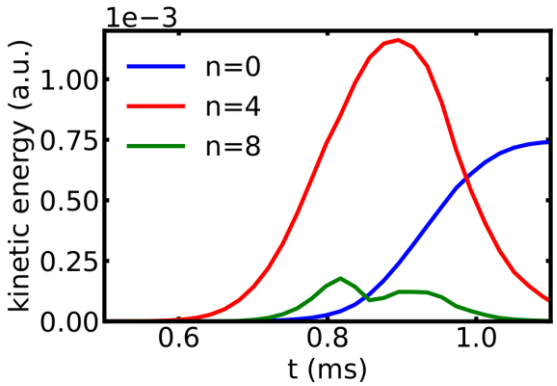

Fig. 2. Nonlinear simulation of saturation of a single Alfvén eigenmode using M3D-C1-K (red line), and the generation of zonal flow (blue line).

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Based on the frequency chirping and the mode-mode coupling simulations, we plan to proceed to study the ALE happening in JT-60, DIII-D and NSTX, which involves an avalanche of a large number of Alfvén modes. This is the most ambitious goal of this project, as it requires a high-accuracy simulation of the abrupt event (in 1ms), and the simulation of the interval between two events (> 10ms) to understand the excitation mechanism. The simulations will be the focus of the project in Year 1 and requires a large amount of computation time. The excited modes can have toroidal mode number *n* ranges from 1 to 10, and frequencies ranging from 10kHz to 100kHz. ALEs happening in JT-60 tokamak have been simulated before using the MEGA code on the Japanese supercomputer JFRS-1 [9], but the simulation was limited to ignore mode-mode coupling and focused on wave-particle resonance, due to the large timescale gap and limitation of computational resources. With our current kinetic-MHD model, we plan to collaborate with NIFS to do a benchmark with MEGA for the JT-60 case. In addition, by utilizing Summit and Frontier, we hope to overcome the previous shortcomings and do full nonlinear simulations of ALEs in DIII-D and NSTX using M3D-C1-K.

Ion kinetic effects in slow MHD instabilities

Except for the high-frequency Alfvén modes, it is found that the kinetic effects of energetic ions or even thermal ions can also play important roles in macroscopic modes with small wavenumbers and frequencies. One of the examples of these modes is the fishbone mode, which is a variant of the MHD kink mode driven by plasma current and localized near the flux surface with a rational toroidal transformation number (*q* value). In the existence of energetic particles, these modes can have a finite frequency and resonate with the precession motion of particles. The new mode is also called non-resonance kink (NRK) mode, since it can be driven without a rational surface, due to the resonance broadening brought by the kinetic effects. Fishbone modes and other other low-frequency MHD modes can also lead to transport of energetic ions in addition to Alfvén modes.

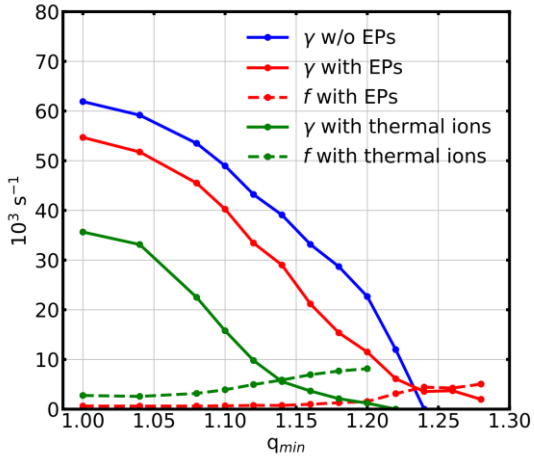

Fig. 3. Growth rates (solid lines) and frequencies (dashed lines) of fishbone modes (red and green lines) compared to pure MHD modes (blue lines), from M3D-C1-K simulation using NSTX parameters.

M3D-C1-K has been used to study fishbone modes in NSTX and DIII-D. We have studied the growth rates and frequencies of the mode with different *q* values through linear simulation (Fig. 3), and in nonlinear simulation we successfully captured the frequency down-chirping of the mode, which is the most important character of fishbone mode in experiments. In this project, we plan to revisit established results and study the stability boundary and plasma beta limit affected by ion kinetic effects. We will also try the extended-MHD simulation which incorporates the two-fluid effects of ion-electron separation, and try to make predictions for ITER.

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Research Objectives of Runaway Electrons

Integrated simulation of MHD instabilities in tokamak disruptions with runaway electron current

It is predicted that in a high-field tokamak-based fusion reactor like ITER, significant runaway electron current can be produced when a disruption event happens. This can change the properties of MHD instabilities in a post-disruption plasma. The MHD modes have been observed in tokamak experiments at DIII-D and JET with deuterium injection to purge high-Z impurities , and has attracted a lot of attention [17].

We have developed a runaway electron module in M3D-C1 which can fit into the mature nonlinear MHD simulation framework for disruption and add the contribution of runaway electron current. In order to overcome the timescale separation between the fast motion of relativistic electrons and the MHD evolution, we applied the method of characteristics to calculate the streaming along the field lines of runaway electrons which can be optimized for GPUs. Using this module, we have done nonlinear simulations for resistive kink instabilities in the DIII-D tokamak. The simulation successfully reproduced the abrupt growth of magnetic perturbation in the post-disruption scenario that happened in the experiment when the edge *q*-value dropped below 2, which resulted in a quick loss of runaway electrons when the magnetic flux surfaces were broken. When runaway electron currents are present, the resistive kink mode can have a large growth rate and a non-zero frequency in the plasma frame, which is consistent with our previous theoretical analysis [18].

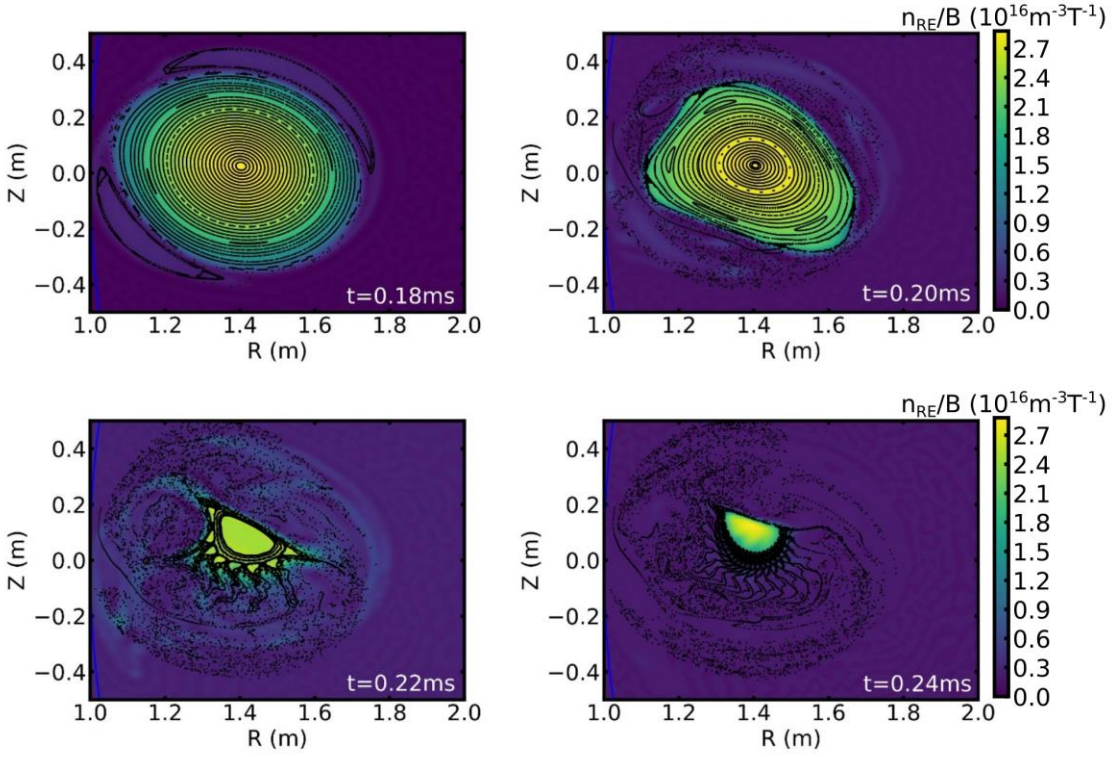

Fig. 3. Loss of runaway electrons (green color) during disruption when magnetic fluxes (black lines) are broken by the excitation of restive kink mode, from M3D-C1-K simulation using DIII-D parameters.

In this project we will use the established module to simulate the entire process of tokamak disruption with runaway electron generation and their interaction with MHD instabilities. This work includes integrated simulation with runaway electron source term, radiation loss of runaway electrons, and other

disruption modules in M3D-C1 like pellet injection. The integrated simulation will be the main focus of the second year of the INCITE project. Note that the injected pellet is strongly localized in the toroidal direction, and to resolve the density and temperature perturbation brought by it and the excited MHD modes, high-resolution 3D mesh is required. The simulation will focus on runaway electron generation location, their impact on plasma facing walls, their survival time in the disruption event, and the efficiency of mitigation strategies. We will also explore alternative mitigation strategies such as RMP and passive coils, which can be more promising for compact tokamak designs like SPARC [19].

Self-consistent simulation current-quench modes driven by runaway electrons

Similar to energetic ions, the high-energy runaway electrons can also drive Alfvén modes or higher frequency whistler modes. These modes have been directly observed in tokamak experiments [20], and are often found to be related to the confinement of runaway electrons [21]. Linear and quasilinear analysis have been applied to study these modes, to understand their impact on runaway electron distribution and their propagation in tokamaks [22]. Recently we upgraded the kinetic module in M3D-C1-K to simulate these electron-driven instabilities. In our simulation we successfully identified the MHz mode observed in DIII-D current quench phase of the disruption as a branch of compressional Alfvén eigenmodes (CAEs) which is driven by the trapped runaway electrons. The nonlinear simulation reveals that subdominant modes with a wide range of frequencies can be driven after the saturation of the initially fastest growthing mode, with strong mode-mode coupling effects.

The simulation of electron-driven current-quench modes is more challenging than ion-driven modes, since the electron velocity is much faster than the ions and the mode frequency is higher (MHz compared to kHz). The simulation thus requires more computation resources and we believe that Summit can be suitable for this job. In this project we plan to use realistic plasma parameters and runaway electron distribution to study the mode excitation criterion, in order to understand the different behavior of RE-driven Alfvén eigenmodes in different experiments. We also plan to extend the current simulation model to study the whistler modes in disruption by including two-fluid effects, which is more challenging as the mode frequency can range from 10MHz to GHz**.**

Research Milestones

Year 1

1. Use the M3D-C1-K code to do nonlinear Alfvén mode simulations with energetic ions, to study the mode frequency chirping and zonal flow generation. We will start with a single mode and extend to multiple modes with mode-mode coupling. We plan to study different scenarios (bursting state and quasi-steady state) in different tokamak experiments including DIII-D and NSTX. This part will take about 20% of the computation time allocated for Year 1 (~ 48,000 node hours).

2. Start nonlinear fishbone simulation using M3D-C1-K with n=1 and extend to higher n to study the difference in their nonlinear behavior. Reproduce nonlinear pressure-driven mode simulations for soft-beta limits and add the ion kinetic effects to it. This part will take about 10% of the computation time allocated for Year 1 (~ 24,000 node hours).

3. Use the M3D-C1-K to do a long-time run for an experimental case with avalanche excitation of multiple Alfvén modes. Study the intermittent excitation and damping of the modes over a longer timescale. Study the effect of collisional and radiation damping of the mode. Compare the results with the MEGA simulation. This part will take about 70% of the computation time allocated for Year 2 (~ 168,000 node hours). It depends on the research work in Milestone 1.

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4. Develop a new GPU version of the particle pushing and MHD matrix calculating by migrating from OpenACC to OpenMP, and test the code on Frontier.

Year 2

1. Complete the electron-driven Alfvén mode simulations by using realistic RE density and energy distribution and plasma parameters. Run longer time nonlinear simulations to study the saturation and damping of the mode. This part will take about 30% of the computation time allocated for Year 1 (~ 72,000 node hours).

2. Set up and run the nonlinear MHD simulation in a disruption scenario with runaway electron current, and enable the RE source term and radiation damping. Analyze the loss of RE when MHD instabilities are present and compare with experimental observations. This part will take about 20% of the computation time allocated for Year 2 (~ 48,000 node hours).

3. Run a fully integrated simulation of a tokamak disruption with runaway electrons and pellect injection, to study the behavior of MHD instabilities in this scenario, the additional generation of runaway electrons due to pellets, and the loss of runaway electrons on walls. Publish the results. This part will take about 50% of the computation time allocated for Year 3 (~ 120,000 node hours). It depends on the research work in Milestone 2.

COMPUTATIONAL READINESS

USE OF RESOURCES REQUESTED

In this project most of the large runs are targeting ALE simulation with multiple Alfvén modes driven by energetic ions, and integrated disruption simulation with runaway electrons and pellet injection, which will be the focus of this project. Both kinds of simulations will run on Summit or Frontier GPU nodes as the energetic particle pushing and MHD matrix calculation are implemented on GPUs. These large runs are critical to the success of the milestones, which have been stated in the section “Research Objective and Milestones”. These runs can only be conducted on large-scale HPC like Summit or Frontier given the scale of the problem and requirement of long simulation time due to timescale separation.

Each large run will employ about 32-128 GPU nodes on Summit, and take about 50-200 hours to finish. The number of nodes are chosen to scale with the number of elements and toroidal planes in the 3D mesh. For Alfvén mode simulations, fine grids in both poloidal and toroidal directions are required given the high wavenumber. In order to simulate waves with frequency around 100 kHz, which is the typical frequency of shear Alfvén modes in a tokamak, a timestep of ~1 microsecond is required. Assuming that the simulation running time of one MHD timestep is 60s, then 200 hours of computation time is required to simulate the evolution of Alfvén eigenmode for 12ms of simulated time, which is the typical time of an ALE [9]. The simulation for MHD instabilities in disruption with runaway electron current typically requires less resources than the Alfvén mode simulation, since the disruption is a relatively faster process and the MHD instabilities have smaller toroidal mode number. However, when doing integrated simulation of disruption including pellet injection, a high-resolution 3D mesh is necessary as the pellet injection can be strongly localized in the toroidal direction, resulting in excitation of multiple modes with different toroidal mode numbers.

Based on the above analysis, we are applying for 480,000 node hours for this 2 year project, 50% for the energetic ion simulation in Year 1 and 50% for the runaway electron simulation in Year 2. These resources will provide us with enough resources for 10-20 large runs for the long-time cases, and will

give us enough opportunities to study the desired cases. As shown in the milestones, we will focus on the some mid-size simulations in the first half of the year to better understand some critical physics issues, and in the second half of the year we will conduct large runs for ALE and integrated disruption simulations, using the knowledge we obtained from the first half of the year. These large runs can give higher burn rates. During this time we will also do data analysis and visualization for the previous simulations and publish the work.

Regarding the data output, the size of an output HDF5 file containing a snapshot of fields and particle information is about 1~8GB, depending on the grid side and the number of particles. For a large run, it takes about 10,000 timesteps and generates about 100 HDF5 files of this size (saving snapshot every 100 timesteps). This data can be simply analyzed using Python on the OLCF clusters. The valuable time step snapshots can be further analyzed using Python, IDL or other tools after transferring the data from OLCF to Princeton University and PPPL clusters. The transfer can be done using rsync or Globus. We expect the data to be stored for 6-12 months on the Filesystem to be used for processing, visualization and publication. After that, the data can be archived to HPSS and saved for future use.

Here are the details on resource requests on simulations in order to reach milestones in each year.

Year 1

1. Use the M3D-C1-K code to do nonlinear Alfvén mode simulations with energetic ions, to study the mode frequency chirping and zonal flow generation. For this work we will conduct 10-20 mid-size runs. Each run will occupy 8-32 nodes with running time about 100 hours, in order to simulate the nonlinear evolution of Alfvén mode in 5-10 ms, which is the characteristic time of Alfvén mode frequency chirping in experiments. The total node hours is about 48,000, which is about 20% of the computation time allocated for Year 1. The generated data will be about 30 TB.

2. Start nonlinear fishbone simulation using M3D-C1-K with n=1 and extend to higher n to study the difference in their nonlinear behavior. For this work we will conduct 10-20 mid-size runs. Each run will occupy 4-16 nodes with a running time of about 100 hours, in order to simulate the nonlinear evolution of fishbone mode in 5-10 ms. The total node hours is about 24,000, which is about 10% of the computation time allocated for Year 1. The generated data will be about 10 TB.

3. Use the M3D-C1-K to do a long-time run for an experimental case with avalanche excitation of multiple Alfvén modes. For this work we will conduct 3-5 large-size runs. Each run will occupy 32-128 nodes with running time about 200 hours, in order to simulate the ALE in tokamak experiments, which has strong excitation of Alfvén modes within 1-2 ms, and intermittency between the excitation about 5-10 ms. The larger number of nodes is necessary for simulation with finer mesh in order to resolve the multiple high-n modes. The simulation will give a high burn rate and we will try to arrange the runs at different times of the year. The total node hours is about 168,000, which is 80% of the computation time allocated for Year 2. The generated data will be about 80 TB.

4. Develop a new GPU version of the particle pushing and MHD matrix calculating by migrating from OpenACC to OpenMP. We will do several tests on Frontier to validate the code and get ready for migration. This part will take only a small amount of node hours (<1,000).

Year 2

1. Complete the electron-driven Alfvén mode simulations by using realistic RE density and energy distribution and plasma parameters. For this work we will conduct 3-5 long-time runs. Each run

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will occupy 8-32 nodes with a running time of about 800 hours. The simulation will give a linear burn rate. The running time is longer because a smaller timestep is required in order to resolve the MHz frequency mode and the motion of relativistic runaway electrons. The total node hours is about 72,000, which is about 30% of the computation time allocated for Year 2. The generated data will be about 50 TB.

2. Set up and run the nonlinear MHD simulation in a disruption scenario with runaway electron current. For this work we will conduct 5-10 mid-size runs. Each run will occupy 4-16 nodes with a running time of about 200 hours. The MHD calculation has similar complexity as the fishbone simulation in Year 1, but the requirement for particle pushing is higher due to the high velocity of runaway electrons, resulting in longer simulation time. The total node hours is about 48,000, which is 20% of the computation time allocated for Year 2. The generated data will be about 20 TB.

3. Run a fully integrated simulation of a tokamak disruption with runaway electrons and pellect injection. For this work we will conduct 5-10 large-size runs. Each run will occupy 32-128 nodes with a running time of about 100 hours. The larger number of nodes is necessary for simulation with finer mesh in order to resolve pellet injection happening in tokamak disruptions which is strongly localized in the toroidal direction. The longer simulation time is because of the higher complexity of the integrated simulation and the required calculation for each timestep. The total node hours is about 120,000, which is 50% of the computation time allocated for Year 3. The generated data will be about 50 TB.

COMPUTATIONAL APPROACH

M3D-C1-K is a hybrid code including a continuum solver for the MHD equations, and a particle simulation module using the PIC method. The MHD equations are discretized using a finite element method on a 3D unstructured mesh, which is generated and managed through the SCOREC library developed at Rensselaer Polytechnic Institute (RPI). The equations are solved as an initial value problem, and advanced in time through full implicit or semi-implicit methods. The time advance matrix is solved using the PETSC library by constructing a block-Jacobi preconditioner and calling GMRES iterative solver. The LU decomposition for each block is obtained using the MUMPS or the SuperLU libraries. The code is mainly developed using Fortran 90, with some new features including function and operator overloading. The interface to the SCOREC and PETSC libraries are developed using C++ with an object oriented model.

M3D-C1-K is composed of three parts, the particle simulation module, the finite element matrix calculation and assembling, and the sparse matrix solver. For each timestep, the MHD fields, including velocite, magnetic fields, and plasma density and temperature, will be used to assemble a new finite element matrix using the Galerkin method. The assembled matrix, together with the field information from the last timestep, is the input to the matrix equation solver which obtains the fields at the new timestep. The field information is also used for the particle orbit and weight calculation. The particle moments, including flow and pressure, will be calculated and deposited on the finite element mesh and used as closure for the MHD equations.

For the MHD part of the simulation, the code has two levels of parallelization. The calculation of the terms of the finite element equation matrix lying on different elements can be done in parallel though MPI or OpenMP. Within an element, the calculation of numerical integral for the test and basis functions in the Galerkin method, which involves summation of contribution from quadrature points, can be done using OpenMP on CPUs or using OpenACC/OpenMP offloading on GPUs. The code can automatically allocate GPU resources for different elements, and allow multiple MPI processes to share a single GPU when

doing matrix calculations using Nvidia's Multi-Process Service (MPS) technique, making the code efficient to run on nodes with multiple GPUs. The matrix is solved using the PETSC library which can run efficiently on multi-core CPUs using MPI and OpenMP.

For the PIC particle simulation part, the code is developed based on a particle-based parallelization model, meaning that the orbit and weight calculation of different particles can run independently on different CPU or GPU threads. We find that this is the most efficient way to do particle pushing on GPUs, as it minimizes the required communication between threads. The particle deposition which involves a reduction calculation of particle moments will run on CPUs using MPI. Note that the particle orbit calculation will run several subcycles between each MHD timestep, and the particle deposition only needs to run once after all the subcycles.

The code uses HDF5 data format to handle I/O. It has two kinds of outputs, one is a small HDF5 file for scalar data, including the global quantities of plasma such as energy and total current. This part will be output every timestep. The other is a larger HDF5 file including all the field and particle information, and will only be output once every 10-100 timesteps. This file can be read using IDL or Python scripts to do post-processing, and can also be used as a snapshot for restart. In addition, the output of M3D-C1-K can be read using the Fusion-IO framework and used by other codes for data processing and visualization. These analyses can be done on OLCF clusters or on the local clusters at PPPL and Princeton University after transferring the data.

Our teams have extensive experience in deploying the code on different architectures and diagnosing issues. We have deployed the code on many HPCs before, including Edison, Hopper, Cori, Perlmutter, and AiMOS. The code can run on different machine architectures including Intel, AMD, IBM and Nvidia using compilers from GNU, Intel, PGI and Nvidia. We have developed tools inside the code to analyze the computation time of each component and find the bottleneck of code running. For the GPU part, we have used diagnostic tools like NSight to further analyze the code efficiency on GPUs. In addition, we are collaborating closely with the LBL team to find the best combination of preconditioner and iterative solver for our matrix.

PARALLEL PERFORMANCE

After finishing the GPU optimization of the particle pushing and MHD matrix calculation modules of M3D-C1-K, we did a benchmark of the code between the CPU and GPU versions to test the performance. The benchmark was done on the Traverse cluster at Princeton University (https://researchcomputing.princeton.edu/systems/traverse), which is a small-scale cluster with 46 computing nodes, and each node has 2 IBM POWER9 32-core CPUs and 4 Nvidia V100 GPUs. The architecture is similar to Summit. The results are shown in Fig .4, and the first result has been published in [13].

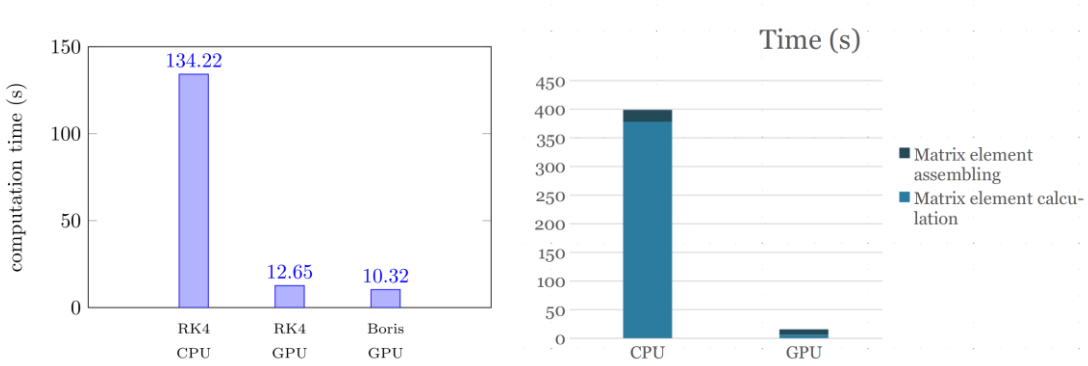

Fig. 4. Speed up of the particle pushing module (left) and matrix calculation module (right) in M3D-C1-K using GPU compared to the CPU version, obtained on Traverse.

Note that these speedup results are obtained by only timing the certain module. There are other components like the iterative matrix solver and the diagnostic calculation (calculation of total energy and plasma currents, etc.) that have not been optimized for GPUs. Fig. 5 shows the computation time for 5 timesteps and one output of snapshot, using 32 nodes on Traverse. We can see that after GPU optimization, the unoptimized parts, especially the matrix solver, become the bottleneck for further speedup. Nevertheless current speedup from GPU optimization is encouraging and can reduce the whole run time by 75%. The further optimization of the matrix solver through the SuperLU library is ongoing, in collaboration with computation scientists from LBL.

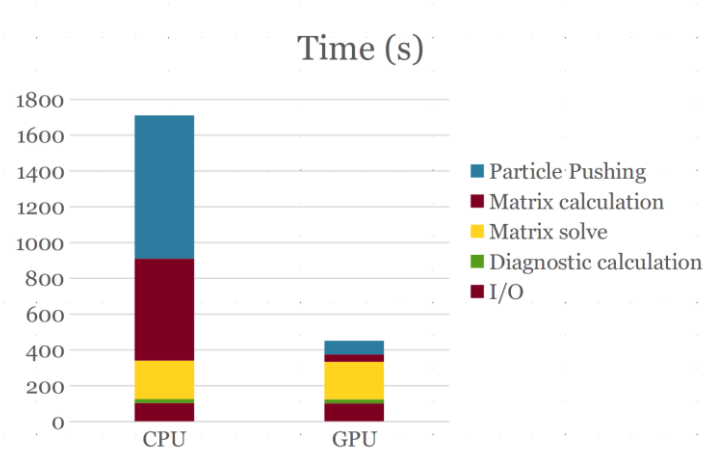

Fig. 4. Comparison of total run time of CPU and GPU versions of M3D-C1-K for 5 timestep, including one snapshot output.

To test the parallel performance of M3D-C1-K code, we chose a test case for a nonlinear simulation of reversed shear Alfvén eigenmode in DIII-D tokamak, and did both weak scaling and strong scaling analysis. The details of the physics setup can be found in [13]. The simulation was conducted on the Traverse cluster. Fig 6 (left) shows the running time of doing 5 timestep calculation on different numbers of nodes, with a mesh of 180,000 elements and 32,000,000 particles. Fig. 6 (right) shows the time spent doing the same simulation when the number of elements in the 3D mesh and the number of particles scale with the number of nodes utilized. Blue lines show the run time excluding the time for I/O.

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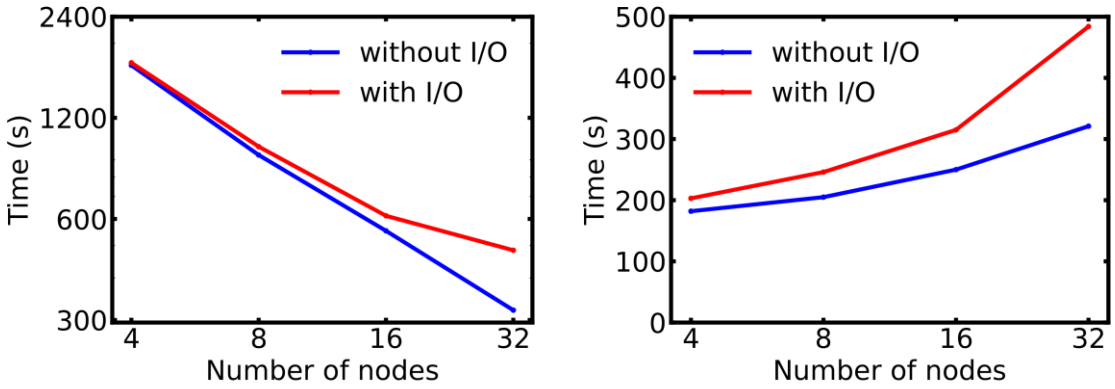

Fig. 6. Strong scaling (left) and weak scaling (right) analyses of parallel performance of M3D-C1-K on Traverse. Blue lines show the computation time without I/O and red lines show the time with snapshot output. In the strong scaling analysis without I/O, the time follows an approximate power law $t \sim N^{-0.807}$.

We find that when excluding the I/O time for snapshot, both the strong scaling and the weak scaling analysis show good overall parallel performance. This means that both the MHD equation solver and the kinetic module have been well optimized for parallel computing. The output of the large HDF5 file for snapshot, however, can become the bottleneck for simulation with a large number of nodes, since the output time can increase as the node number increases, which is different from other components of the code. Therefore for runs employing a large number of nodes, we need to decrease the frequency of the snapshot output, and rely more on the scalar output which takes only ignorable time.

DEVELOPMENTAL WORK

To make the M3D-C1-K code suitable for running on Summit, we have developed GPU optimization for two modules of the code. The particle pushing module can run efficiently on GPUs and has been tested on Summit and Traverse, which can also be used for the runaway electron simulation. The matrix calculation part has been restructured recently to fit the requirements for GPU optimization, by separating the physics part and the numerical integration part. The numerical integration part has been ported to GPU using OpenACC, which is also available for the Nvidia compiler on Summit.

During this project, we plan to test different arrangements of number of processes, threads, and GPU threads allocation, to find the most efficient strategy to run the M3D-C1-K code on Summit. One of the challenges we have found for running the code on other HPCs is the high requirement of memory of the matrix solver, which can limit the number of processes we can have per node. Therefore for Summit we plan to collaborate with the PETSC developers, OpenMPI developers, and SuperLU developers to solve this issue and improve the efficiency of the simulation.

We plan to migrate to the Frontier cluster from Summit after FY2023. This requires us to change the OpenACC GPU directives, which is only supported by Nvidia GPUs, to the OpenMP directives with GPU offloading, which is supported by AMD and Intel. We have tested the OpenMP offloading in the particle-pushing module of the M3D-C1 code using IBM XL compiler on Nvidia GPUs, and have reached satisfying results. For FY 2023, we are applying for 10,000 nodes hours on Frontier in order to test the OpenMP version of the GPU code using AMD ROCm/AOMP compiler. This will enable us to

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have a smooth transition from Summit to Frontier, and will better prepare us for future clusters with different architectures.

In addition, we plan to develop new functions and improve the efficiency of the kinetic module for energetic ions and runaway electrons. For energetic ions, we will develop a collisional operator including the slowing-down and pitch angle scattering calculation, which is necessary for the long-time ALE simulations in the Year 2 milestone. This work will be conducted in Year 1 and will be validated through benchmarking with the MEGA code, which already has a collisional operator. For the runaway electrons, we will test the compatibility of this module in our existing disruption simulation of VDE and pellet injection, in order to do the integrated simulation for the tokamak disruption in the Year 3 milestone. In addition, we will test GPU programming models other than OpenACC, such as OpenMP offloading and HIP (by applying for an account on Crusher), in order to prepare the code for future deployment on Frontier and other HPCs.

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PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

- Stephen Jardin is a principal research physicist at the Princeton Plasma Physics Laboratory. Stephen is one of the primary developers of M3D-C1(with Nathaniel Ferraro). He is the Principal Investigator of the SciDAC "Center for Tokamak Transient Simulation (CTTS)". He has taught a graduate course on "Computational Methods in Plasma Physics" at Princeton University for 25 years and has authored a textbook of the same name (Taylor and Francis, 2010). He is a Fellow of the American Physical Society. He is one of the 2 U.S. representatives to the ITER ITPA committee on Disruptions, MHD, and Plasma Control. Steve will use his experience to provide support for the development of M3D-C1-K, including the finite element method and the implicit solver, and will also help on the physics analysis of MHD instabilities, especially those of concern to ITER.

- Amitava Bhattacharjee is a Professor of Astrophysical Sciences at Princeton University. He has taught previously at Columbia University, the University of Iowa and the University of New Hampshire. He has received the James Van Allen Natural Sciences Fellowship, the Faculty Scholar Award, and the Michael J. Brody Award. He is a Fellow of the American Physical Society, the American Association of the Advancement of Science, and the American Geophysical Union. Amitava is one of the co-PIs of the SciDAC "Simulation Center for Runaway Electron Avoidance and Mitigation (SCREAM)". He has been the PI of several INCITE projects before. He will use his experience to support the management of this project, and give insights on the explanations of the physics findings.

- Jin Chen is a computational scientist at Princeton Plasma Physics Laboratory. Jin has extensive experience on development of several codes, including M3D, GTS, and M3D-C1. She is an expert on the PETSC matrix solver library which is an important component of the M3D-C1 code. In this project Jin will use her knowledge to support the development and optimization of the PETSC solver and GPU optimization.

During this 3-year project we plan to hire 1-2 postdocs and invite graduate students and summer students to join the project. The postdocs and students will use Summit as a platform to learn about HPC and M3D-C1-K code through practicing. They will also do some small to medium scale simulation runs depending on their interests. In addition to current personnel, we also have wide collaborations with people from the theory and computational science department at PPPL, and we may invite more people to join this project in future.

MANAGEMENT PLAN

The PI of the project (Chang Liu) will be responsible for most of the simulation work and thus take most of the allocation time. Chang will make a decision of the allocation between the two subprojects, the kinetic ion simulation and runaway electron simulation. The M3D-C1 team at PPPL will have bi-weekly meetings to discuss the development of the code and usage of the allocated computation time, and Chang will present the current usage trend to all the team members and ask for suggestions. Stephen, Amitava and Jin will provide support on both the physics and computational side regarding the project, in order to reach the milestones in time. Chang Liu (cliu@pppl.gov) will be the contact and be responsible to report the progress of the project, including publication and awards, and be responsible for the future renewal of the project.

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Proposal Title (exactly as it appears on submission): Hybrid simulation of macroscopic instabilities with energetic particles in fusion plasma

Year 1		**Total number of node-hours for Year 1:** 240,000	
Milestone:	**Details (as appropriate):**	**Dates:**	**Status: (renewals only)**
1. Study the mode frequency chirping and zonal flow generation in nonlinear Alfvén mode simulation.	**Resource:** Summit **Node-hours:** 48,000 **Production size runs (number of nodes):** 8-32 **Filesystem storage (TB and dates):** 30 TB, 01/01/2023-03/31/2023 **Archival storage (TB and dates):** 30 TB, 2023 **Software Application:** M3D-C1-K **Tasks:** Run nonlinear simulations of a single Alfvén mode using M3D-C1-K to obtain the chirping rate and analyze the particle distribution evolution. Analyze the dependence of zonal flow generation on plasma and energetic ion conditions **Dependencies:** None	01/01/2023-03/31/2023	
2. Start nonlinear fishbone simulation using M3D-C1-K. Reproduce nonlinear pressure-driven mode simulations for soft-beta limits and add the ion kinetic effects to it.	**Resource:** Summit **Node-hours:** 24,000 **Production size runs (number of nodes):** 4-16 **Filesystem storage (TB and dates):** 10 TB, 04/01/2023-04/31/2023 **Archival storage (TB and dates):** 10 TB, 2023 **Software Application:** M3D-C1-K **Tasks:** Conduct nonlinear simulation of n=1 and higher n fishbone mode simulation. Study soft-beta limit with ion kinetic effects **Dependencies:** None	04/01/2023-04/31/2023	
3. Study avalanche excitation of multiple Alfvén modes in ALEs. Study the intermittent excitation and damping of the modes over a longer timescale. Study the effect of collisional and radiation damping of the mode.	**Resource:** Summit **Node-hours:** 168,000 **Production size runs (number of nodes):** 32-128 **Filesystem storage (TB and dates):** 80 TB, 05/01/2023-12/01/2023 **Archival storage (TB and dates):** 80 TB, 2023 **Software Application:** M3D-C1-K **Tasks:** Use M3D-C1-K to do long-time simulation of multiple Alfvén mode excitation. Run a similar simulation using MEGA and compare the results.. **Dependencies:** Milestone 1 of Year 1	05/01/2023-12/01/2023	
4. Develop a new GPU version of the particle pushing and MHD matrix calculating, and test the code on Frontier.	**Resource:** Frontier **Node-hours:** 1,000 **Production size runs (number of nodes):** 4-16 **Filesystem storage (TB and dates):** 1 TB, 12/01/2023-12/31/2023 **Archival storage (TB and dates):** 1 TB, 2023 **Software Application:** M3D-C1-K	12/01/2023-12/31/2023	

	Tasks: Change the GPU directives in the M3D-C1-K code from OpenACC to OpenMP and test the new code running on Frontier **Dependencies:** None		
Year 2		**Total number of node-hours for Year 2:** 240,000	
1. Complete the electron-driven Alfvén mode simulations. Run longer time nonlinear simulations to study the saturation and damping of the mode.	**Resource:** Summit **Node-hours:** 72,000 **Production size runs (number of nodes):** 8-32 **Filesystem storage (TB and dates):** 50 TB, 01/01/2024-04/01/2024 **Archival storage (TB and dates):** 50 TB, 2024 **Software Application:** M3D-C1-K **Tasks:** Conduct nonlinear current quench mode simulation driven by runaway electrons, study how the modes affect the diffusivity of RE beams **Dependencies:** None	01/01/2024-04/01/2024	
2. Study runaway electron generation and loss in tokamak disruption with significant MHD modes excited.	**Resource:** Frontier **Node-hours:** 48,000 **Production size runs (number of nodes):** 4-16 **Filesystem storage (TB and dates):** 20 TB, 04/01/2024-07/01/2024 **Archival storage (TB and dates):** 20 TB, 2024 **Software Application:** M3D-C1-K **Tasks:** Conduct nonlinear MHD simulation with RE current for a DIII-D or JET experimental case, add the RE source term and radiation energy loss, study the coupling between RE current MHD instabilities. **Dependencies:** None	04/01/2024-07/01/2024	
3. Do integrated simulations of tokamak disruptions with runaway electrons and pellect injection. Publish the results.	**Resource:** Frontier **Node-hours:** 120,000 **Production size runs (number of nodes):** 32-128 **Filesystem storage (TB and dates):** 50 TB, 07/01/2024-12-31-2024 **Archival storage (TB and dates):** 50 TB, 2024 **Software Application:** M3D-C1-K **Tasks:** Integrate the developed RE model and source term with the established disruption simulation model with pellet injection. Run the simulation with all the key physics, and compare the obtained RE generation loss rate with experiments. **Dependencies:** Milestone 2 of Year 2	07/01/2024-12/31/2024	

Curriculum Vitae
Chang Liu
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PROFESSIONAL PREPARATION

PhD 2011-2017
Astrophysical Sciences, Program in Plasma Physics, Princeton University, Princeton, USA

Bachelor of Science 2007-2011
Physics, Peking University, Beijing, China

APPOINTMENTS

2019–present Staff Research Physicist at Princeton Plasma Physics Laboratory

2017-2019 Associate Research Physicist at Princeton Plasma Physics Laboratory

FIVE PUBLICATIONS MOST RELEVANT TO THIS PROPOSAL

1. C. Liu, S.C. Jardin, H. Qin, J. Xiao, N.M. Ferraro, and J. Breslau, "Hybrid simulation of energetic particles interacting with magnetohydrodynamics using a slow manifold algorithm and GPU acceleration", Computer Physics Communications **275**, 108313 (2022).
2. C. Liu, S.C. Jardin, J. Bao, N. Gorelenkov, D.P. Brennan, J. Yang, and M. Podesta, "Thermal ion kinetic effects and Landau damping in fishbone modes", arXiv:2206.03648 (2022).
3. C. Liu, C. Zhao, S.C. Jardin, N.M. Ferraro, C. Paz-Soldan, Y. Liu, and B.C. Lyons, "Self-consistent simulation of resistive kink instabilities with runaway electrons", Plasma Phys. Control. Fusion **63**, 125031 (2021).
4. C. Liu, D.P. Brennan, A. Lvovskiy, C. Paz-Soldan, E.D. Fredrickson, and A. Bhattacharjee, "Compressional Alfvén eigenmodes excited by runaway electrons", Nucl. Fusion **61**, 036011 (2021).
5. C. Liu, E. Hirvijoki, G.-Y. Fu, D.P. Brennan, A. Bhattacharjee, and C. Paz-Soldan, "Role of Kinetic Instability in Runaway-Electron Avalanches and Elevated Critical Electric Fields", Phys. Rev. Lett. **120**, 265001 (2018).

RESEARCH INTERESTS AND EXPERTISE

- Alfvén instabilities driven by energetic particles
- Magnetosonic-whistler instabilities excited by runaway electrons in tokamak disruptions
- Runaway electron physics in flattops and disruptions in tokamaks
- High-order gyrokinetic theory for relativistic electrons
- GPU optimization for finite-element codes

SYNERGISTIC ACTIVITIES

1. Invited talk at the 30th International Toki Conference (2021)
2. Invited talk at the 63rd Annual Meeting of the APS Division of Plasma Physics (2021)
3. Invited talk at the 5th Asia Pacific Conference on Plasma Physics (AAPPS-DPP) (2021)
4. Invited talks at Theory and Simulation of Disruption Workshop 2021
5. Invited talk at Runaway Electron Meeting (REM) 2018

COLLABORATORS (*PAST 5 YEARS INCLUDING NAME AND CURRENT INSTITUTION*)

Stephen Jardin, Princeton Plasma Physics Laboratory

Amitava Bhattacharjee, Princeton Plasma Physics Laboratory
Nathaniel Ferraro, Princeton Plasma Physics Laboratory
Nikolai Gorelenkov, Princeton Plasma Physics Laboratory
Chen Zhao, General Atomics
Dylan Brennan, Princeton University
Carlos Paz-Soldan, Columbia University
Guillaumme Brochard, University of California Irvine
Zhihong Lin, University of California Irvine

Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

M3D-C1

Indicate whether Open Source or Export Controlled.

Export Controlled

Package Name

SCOREC

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

PETSC

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

HDF5

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

Yes

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

Question #2

Suggested Reviewers

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

testbedresources.pdf
The attachment is on the following page.

Testbed Resources

We are interested in developing a new solver for the MHD equation in our code based on AI/ML techniques. The machine learning techniques have been used as surrogates for traditional numerical simulation codes in order to reduce the computation time and accelerate the categorization work for large amounts of data. We propose to use a different strategy, which is to use ML to accelerate the semi-implicit operator in our MHD simulation code.

The semi-implicit operator was introduced as an alternative to the fully implicit time integration method. In the fully implicit method, it is necessary to solve the implicit equation with a large singular sparse matrix including all the fields, which can be computationally expensive. With the semi-implicit operator, the time evolution equations of velocity and magnetic fields can be solved separately, and the operator can help suppress numerical instabilities when the Courant–Friedrichs–Lewy (CFL) condition is violated. However, for complicated magnetic fields like those in tokamaks and stellarators, the operator itself can be complicated and the evaluation and LU decomposition of it can be difficult. It has been found that for GPU machines the calculation and solving of this operator can be the bottleneck of further optimization of the code. Thus we propose to use ML to do the job of this operator, which is to damp the numerical modes driven by the split time integration method, while keeping all the physics modes untouched. If it works, we can then use the several AI/ML accelerators available at ALCF testbeds to further accelerate our codes and reach a computation efficiency similar to that of explicit method, but without limitation of CFL condition.