2023 INCITE Proposal Submission
Proposal

Title: First-principles Simulations of Pulsar Magnetospheres
Principal Investigator: Revathi Jambunathan
Organization: Lawrence Berkeley National Laboratory
Date/Time Generated: 6/17/2022 5:38:27 PM

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.*

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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.*

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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

Pulsars are rapidly rotating, highly magnetized neutron stars that emit electromagnetic radiation at a regular
period. However, their emission mechanism is still a mystery. The proposed ab-initio simulations will unveil the
dominant emission sites, structure, and composition of the magnetosphere, and probe the fundamental
processes that drive high-energy emissions.

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

2019

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

My five-year research objective is to couple continuum-kinetic methods such that both large-scale
pulsar-wind and small-scale plasma kinetics in the magnetosphere can be captured self-consistently. Observations of the Crab nebula indicate that the pulsar at its center powers the
nebula's magnetic fields and high-energy radiation. It is in just this regime that the continuum
approximations of magnetohydrodynamics (MHD) capture interactions between the pulsar wind
and the surrounding nebula. The proposed fully-kinetic Particle-In-Cell (PIC) simulations of pulsar
magnetospheres will uncover the structure of the magnetosphere and provide physical insight into
the fundamental processes that drive emission.
The proposed fully-kinetic simulations of pulsar magnetospheres align with the research objectives in two
aspects :
1. They provide detailed information on the interaction between charged particles and strong
electromagnetic fields in the pulsar magnetosphere required to extract physical insight on

fundamental acceleration mechanisms
2. We will leverage advanced numerical strategies and use mesh-refinement with electromagnetic PIC to bridge disparate length scales in the pulsar magnetosphere simulations.

These two components will form the framework for expanding and building a self-consistent MHD-PIC model to capture large-scale dynamics driven by the microscale processes in the equatorial current-sheet of pulsars. The insights gained from the detailed PIC simulations will also form the basis of sub-grid models that can be used in larger-scale MHD simulations. The methods developed can also be extended to model black-hole magnetospheres and accretion disks expanding our understanding of our known universe.

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

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Node Hours

255,540

Storage (TB)

4,900

Off-Line Storage (TB)

2,200

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

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 X^e) 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

DOE Base Math Program (for algorithmic development)

Grant Number

Simulation and Analysis of Reacting Flow, FWP # FP00011940, Funded by Applied Mathematica Program in ASCR

Funding Source

Exascale Computing Project (ECP) (leveraged by using ECP-code WarpX)

Grant Number

17-SC-20-SC

Question #13

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

Other High Performance Computing Resource Allocations

Resource

Perlmutter

Allocation Agency

National Energy Research Scientific Computing Center (NERSC)

Allocation

10,000 nodes hours on perlmutter

Allocation Year

2021-2022

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.**

INCITE_2023_AstroPlasmaWarpX_RJ.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: First-principles Simulations of Pulsar Magnetospheres

PI and Co-PI(s): Revathi Jambunathan, Hannah Klion, Andrew Myers, Michael Rowan, Jean-Luc Vay, Weiqun Zhang

Applying Institution/Organization: Lawrence Berkeley National Laboratory

Number of Processor Hours Requested: 255,540 Node-hours on Frontier

Amount of Storage Requested: 4,900 PB (long-term), 2,200 TB (short-term)

Executive Summary:

Pulsars are some of the most intriguing objects in our known universe. They are highly magnetized, rapidly rotating neutron stars that emit electromagnetic radiation. Pulsars were known to emit radiation in the long-wavelength radio to very short-wavelength, high-energy, X-ray spectrum. However, the 2010 detection of gamma ray flares from pulsars challenged the widely accepted understanding of emission mechanisms, which could not explain the flares above 160 MeV. Understanding the interactions of charged particles with extremely high electromagnetic fields is critical to gaining insight on pulsar emission.

The precise timing of pulsar signals has led to the discovery of exoplanets, indirect detection of gravitational waves, study of quantum processes in a strong magnetic field, and in pulsar timing arrays for navigation, yet their emission mechanism is still a mystery. Therefore, computational simulations are essential for studying the microphysics that drive particle acceleration and identifying emission sites in the region surrounding pulsars, called the magnetosphere. The ratio of physical length scales that span pulsar magnetospheres is on the order of a million. However, even with the world's most powerful supercomputers, it is infeasible to simultaneously resolve the local acceleration mechanisms and capture the global plasma dynamics in a single simulation.

We propose a comprehensive set of electrodynamic Particle-In-Cell (PIC) simulations using a wide computational lens to study global characteristics, namely, plasma composition, structure, and energy dissipation as well as pulsar spindown; and also use a focused lens to zoom-in to the current-layer in the magnetosphere, which is an ideal site for reconnection-driven particle acceleration. For all our simulations, we will use the Exascale Computing Project electromagnetic PIC code WarpX that has a proven track record for high-fidelity modeling of relativistic plasma processes. We will leverage advanced numerical algorithms, specifically the ultra high-order spectral solver and the near-ideal scaling performance of the GPU-optimized code, to resolve large scale separations inherent to pulsar magnetospheres. We will perform three-dimensional relativistic magnetic reconnection simulations to study the evolution of flux ropes, particle acceleration, and effect of guide field for a magnetization representative of a realistic pulsar system. We will quantify the energy transfer from the magnetic field to particle heating and acceleration. We will also perform global pulsar magnetosphere simulations to study the influence of the artificial reduction in scale-separation typically used in PIC simulation on the spindown, energy dissipation predictions, and particle energization in the equatorial current-sheet. We will also perform simulations with different plasma injection rates to study its effect on the global structure, composition and plasma trajectory in the pulsar magnetosphere. To our knowledge, these will be the first simulations of three-dimensional pulsar magnetospheres with a spectral solver for a scaling of $R^*/\lambda_{\mathrm{sd}}$=100 and will form a significant contribution to the astrophysical plasma community.

The particle energy spectra from our simulations will be compared with measured emission spectra to benchmark our computational results. The physical insight gained from resolving the fundamental acceleration mechanisms can provide a basis for developing sub-grid models to be used in larger-scale magnetohydrodynamic simulations. Any additions made to the code will also be useful for study other relativistic plasma processes, such as relativistic shocks, and accretion discs, and thus a contribution to the wider plasma community.

PROJECT NARRATIVE

1 SIGNIFICANCE OF RESEARCH

Pulsars are highly magnetized, compact (10–15 km in radius) neutron stars which spin rapidly, 7–700 times a second. This unique combination leads to strong electromagnetic radiation, the cause for which is still not well understood. Until 2010, the energies detected from pulsar emission were approximately 25 GeV or less[2]. However, in 2010, the Fermi Large Area Telescope (LAT)[1, 3] and the Cherenkov Telescope Array (CTA)[2] detected very high energy gamma ray flares ($\gtrsim$ 100 GeV) from the Crab pulsar (PSR J0534+2200). These observations challenged the widely accepted understanding of emission mechanisms, rooted in ideal plasma physics, that had been successful in explaining low energy observations. The paradigm-challenging observations suggest that non-ideal processes likely play an important role in driving rapid particle acceleration and the associated very high energy emissions. Fully kinetic simulations are required to model these non-ideal processes. First principles particle-in-cell (PIC) simulations are necessary to fully probe the non-ideal plasma kinetics that mediates particle acceleration and the subsequent high energy electromagnetic radiation. However, the length-scale separation between the near-surface plasma skin-depth and the size of the pulsar magnetosphere region containing current-sheets is at-least six orders of magnitude. As a result, to enable the study of such large-scale systems, kinetic simulations are typically performed for a scaled-down magnetic field-strength, such that the scale-separation in the system is smaller than the realistic system. Consequently, many kinetic processes, such as pair-production and radiation reaction that are present in strong magnetic field systems, are typically not self-consistently included in scaled-down global simulations. Instead, a multiplicity factor is used to artificially increase the effective magnetic field strength, determine the cooling rate caused by radiation processes, and study its effect on particle acceleration. **In this simulation campaign, we propose to extend the current state-of-the-art by increasing the scale separation between plasma kinetics and the pulsar to at-least 400 for a three-dimensional study with enough resolution for the skin-depth and large domain-size (nearly 20× pulsar radius).** To do so, we will leverage the advanced numerical algorithms and near-ideal scaling performance of the GPU-optimized, electromagnetic PIC code WarpX [32, 22] to resolve large scale-separations inherent to pulsar magnetospheres. Using the ab initio kinetic simulations proposed in this campaign, we will probe both global dynamics and local kinetics of the pulsar magnetosphere, which will unveil answers to the specific questions below and form critical pieces of the much larger pulsar emission puzzle:

- Where in the magnetosphere are plasma particles accelerated, and how is electromagnetic energy dissipated?
- How do these microphysical processes affect the large-scale spindown rate and Poynting flux of the pulsar magnetospere?
- What is the effect of artificially scaling down the magnetic-field strength in numerical simulations on the predictions of spindown rate?
- How much energy is transferred from the field to heating and non-thermal acceleration of particles?

The results from our simulations will contribute to some of the open questions relevant to high-energy emission from pulsar systems and the often-invoked magnetic reconnection in such systems[18]. The fully-kinetic, 3D, PIC simulations of global pulsar magnetospheres proposed in this work will enable us to investigate locations of non-thermal particle acceleration, while still capturing global quantities such as Poynting flux, energy-dissipation, and spindown rate. Even with all the resources on the most-advanced leadership class computing facilities, studying a realistic pulsar magnetosphere is intractable due to large scale separations that span it. Therefore, the global plasma dynamics in a pulsar magnetosphere have to be studied with multiple apertures to study both global dynamics and resolve local plasma kinetics. So, in addition to performing global pulsar magnetosphere simulations for a scaled-down system, we will also probe reconnection in the current sheet layer for a relativistic magnetic field strength, to further our understanding on how energy is transferred from electromagnetic fields to high-energy plasma particles.

As part of a DOE-funded Base Math project, this simulation campaign is critical to developing a hybrid continuum-kinetic approach recognized as one of the key developments required to link microscale physics with macroscale observations[18]. Although originally motivated by astrophysical plasma, the insights obtained from our first principles kinetic simulations may also apply to reconnection for Earth-bound applications such as fusion devices[34] and some of the planned experiments with FLARE (Facility for LAboratory Reconnection Experiments)[18, 17] and TREX (Terrestrial Reconnection EXperiment)[13].

To meet our research objectives, we will perform first-of-its-kind, ultra-high order, pseudo-spectral analytical time domain (PSATD) [31, 33] PIC simulations, which are known to be less susceptible to numerical dispersion effects than the widely-used finite-different time domain (FDTD) [29] methods [14, 4]. Although our preliminary studies show the FDTD and PSATD produce the same results, we have found that the PSATD method is still faster, due to the 1.7 times larger timestep. We will leverage the advanced numerical algorithms and capabilities of WarpX, an electromagnetic Particle-in-Cell Exascale Computing Project (ECP) code. The code is optimized to perform large scale simulations on leadership class computing facilities with near-ideal scaling performance[22]. With this highly efficient code, we will perform global pulsar magnetosphere simulations and also zoom-in to the current sheets, and capture the detailed particle kinetics along with large-scale tearing-mode and drift-kink instabilities, and we will also zoom-out to perform global simulations of pulsar magnetospheres.

1.1 Global Pulsar Magnetosphere Simulations

Fully-kinetic simulations of global pulsar magnetospheres are crucial to understanding the plasma composition, structure, and particle acceleration. Accurate modeling of the kinetic effects using PIC requires resolution of the skin depth at the surface of the pulsar as well as of the current sheet, while also modeling a significant region beyond the light cylinder to study the current sheet kinetics there. For a realistic pulsar, the skin-depth, λ_{sd}, is six orders of magnitude smaller than the radius of the star, R^*, which is a fraction of the light-cylinder [23]. Thus, resolving the charge density at the pulsar surface while also capturing global dynamics in the magnetosphere for a physically realistic system is intractable with a uniform grid method due to limitations of computational capabilities and hardware. Therefore, instead of using the actual value of $\frac{R_*}{\lambda}$=10^6, the skin-depth is scaled in PIC simulations by decreasing the magnetic field strength, such that, $\frac{R_*}{\lambda}$=10-10^2. Previous works on global pulsar magnetosphere simulations have studied the plasma structure, composition, effect of pair-production or rate of plasma-injection and general relativity[5, 24, 25, 19, 8]. However, a detailed analysis on the effect of scaling down the magnetic field strength is not available. Additionally, 3D simulations with 400× difference in length-scales, such that, plasma skin-depths are well-resolved, have not been studied. The main objectives of our simulation campaign are

(a) to study the effect of scaling down the magnetic field, and injection rate on the structure and composition of pulsar magnetosphere for oblique pulsars
(b) to probe the main acceleration sites in the magnetosphere, and
(c) quantify the luminosity, dissipation rate, and spindown rate of the pulsar.

The main physical modules required to achieve this objective include (1) conducting boundary condition [25, 19] (2) surface-charge injection as well as pair-formation to fill the magnetosphere [8, 25]. We implemented these modules in WarpX and performed preliminary 3D PIC simulations for an aligned pulsar. For a realistic system, plasma-pair is produced by quantum-electrodynamic (QED) processes. However, for scaled-down simulations, the magnetic field is much lower than the threshold Schwinger field in order to self-consistently account for pair-production. As a result, many studies inject plasma if the local magnetization is greater than a threshold value in order to model the pair-production process. Since plasma density in pulsars range from low-density (inactive pulsars) to dense (active pulsars), studying the rate of injection becomes important. While one group has studied these effects, the study in 3D has not been performed for a scaling ratio of 400, with the resolution that we have proposed in our simulation campaign.

We performed preliminary studies with two extreme injection rates, namely, $0.2F_{GJ}$ to study low-density vacuum solutions, and $5F_{GJ}$ to study plasma-filled magnetospheres, where, F_{GJ} is the Goldreich-Julian plasma flux at the surface[21]. The total charge density variation extracted on a slice along the rotation axis (y-z plane) and across the rotation axis (x-y) are shown in Figs. 1 and 2, respectively. It can be seen that the low injection rate leads to a charge-separate disc-dome solution with electrons trapped near the magnetic poles and positrons forming a disc near the equator and signatures of the diocotron instability can be seen in Fig. 2. Increasing the rate of injection to $5F_{GJ}$ results in the formation of current-sheet in the equatorial plane that extends beyond the light cylinder, located at 48 km. The top-view of this region, shown in Fig. 4, demonstrates the spiral feature of the current sheet as is expected for the aligned case. The scaling ratio in these simulations is 20× smaller than the proposed baseline simulation and 70× smaller than the largest scaling ratio we propose. The proposed simulations will be performed for an oblique pulsar, which has also been implemented and tested, such that the skin-depth is well-resolved in the current-sheet and everywhere in the light-cylinder. Global pulsar magnetosphere simulations have not been studied at this scale for an oblique pulsar in 3D and this multiplicity (injection rate), and thus we propose to carefully examine the effect of scaling and injection rate.

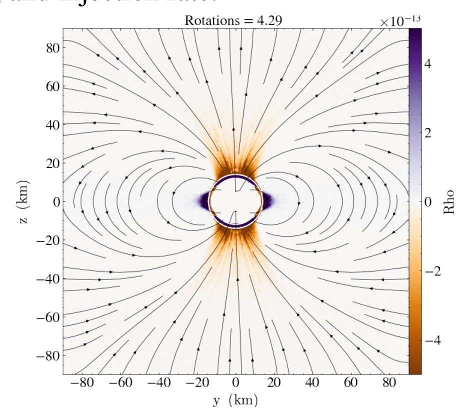

Figure 1. Charge-separated electrosphere (disc-dome) solution in a sample 3D global pulsar magnetosphere simulation with an injection rate of $0.2F_{GJ}$ [16].

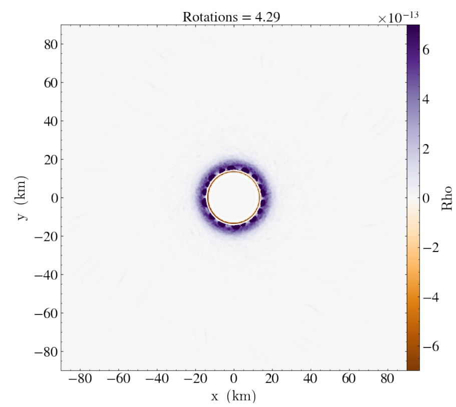

Figure 2. Equatorial plane of an aligned pulsar with injection rate of $0.2F_{GJ}$ exhibiting signatures of diocotron instability [16].

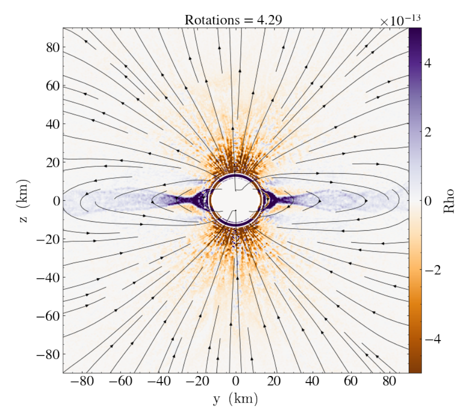

Figure 3. Plasma-filled magnetosphere for an aligned pulsar with injection rate $5F_{GJ}$. Unlike the vacuum solution (Fig. 1), a current-sheet forms and extends beyond the light cylinder (R=48 km) [16].

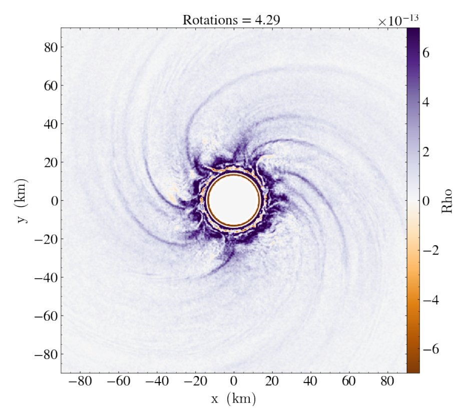

Figure 4. Top-view of the equatorial current-sheet for an injection rate of $5F_{GJ}$, which shows plasma forming a spiral as the pulsar spins around its axis [16].

Since we scale down the magnetic field strength in global pulsar magnetosphere simulations, we will "zoom-in" to the current sheet shown in Figs. 3 and 4 to probe the local physics in this region for a realistic magnetic field strength. Magnetic reconnection simulations of the current sheet will enable us to uncover the kinetic mechanisms that cause rapid particle acceleration, and is discussed in the next section.

1.2 Relativistic Magnetic Reconnection

Magnetic reconnection is a fundamental plasma physics process that converts magnetic energy to particle kinetic energy. The conditions required for magnetic reconnection (i.e. flux freezing and a mechanism to drive the formation of X-points) are easily met in a variety of astrophysical systems, including Earth's magnetosphere, the solar atmosphere, black hole coronae, and jets of active galactic nuclei, among others [18]. Numerous PIC studies have demonstrated the capability of magnetic reconnection to generate high-energy particles, thus it is often invoked to explain the high energy emissions observed in astrophysical contexts where reconnection can occur. While there are several PIC studies focused on pulsar magnetospheres[6, 8, 24, 25], these are designed to capture plasma dynamics at scales comparable to the pulsar radius, which is many orders of magnitude larger than the microphysical length scales at which magnetic reconnection is adequately resolved. As a complement to our global simulations of pulsar magnetospheres, we plan also to study the microphysics of reconnection in pulsar magnetospheres. While there is a theoretical expectation that reconnection in pulsar magnetospheres proceeds in the relativistic regime [10, 30], we will be able to test this expectation by examining the magnetizations (i.e. $\sigma \equiv B_0^2/(\mu_0 n m_e c^2)$, where B_0 is the magnitude of the alternating component of magnetic field, n is the local number density, m_e is the mass of the electron, μ_0 is the vaccuum permeability, and c is the speed of light; this expression is given in SI units) and guide field (i.e. B_g, the out-of-plane component of magnetic field) achieved in our global simulations of pulsar magnetospheres, thus providing a first-principles justification for the upstream magnetization and guide field in our reconnection simulations.

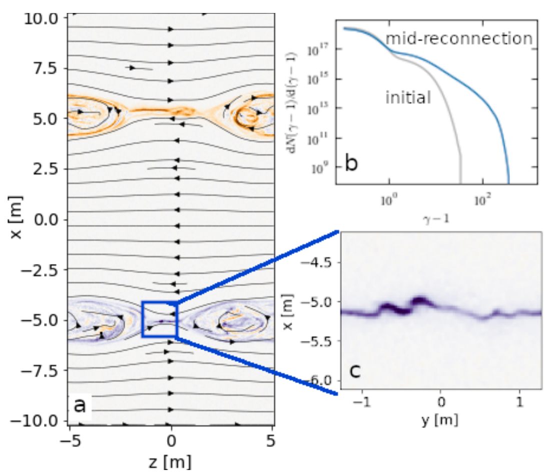

Figure 5. Pilot 3D simulations of relativistic magnetic reconnection. Panels (a) and (c) show the current density in the two planes perpendicular to the current sheets. Panel (a) shows the plasmoid structures that form due to the tearing-mode instability, and panel (c) shows the drift-kink instability, which causes deformation in the current sheet. Panel (b) shows the particle energy distributions initially (gray) and mid-reconnection (blue), showing that particles are accelerated by reconnection.

These micro-scale simulations of reconnection will allow us to probe the capacity of reconnection, in the context of pulsar magnetospheres, to produce high energy emissions, and to examine the mechanisms responsible for producing high-energy particles. Due to the inherently 3D nature of pulsar current sheets, and the potentially stochastic non-linear 3D dynamics of reconnection from the drift-kink instability [7, 15, 28, 36], we choose to run our zoomed-in simulations in 3D. Motivated by results in our pilot global simulations of pulsar magnetospheres, we adopt for our 3D reconnection simulations (described in detail in Secs. 2.1 and 2.2) a magnetization $\sigma = 30$, and a range of guide fields $B_g = 0.25B_0, 0.5B_0$, and $1.0B_0$; in Fig. 5, we show results from a pilot 3D simulation of reconnection, including (panel a) current density, (panel b) time evolution of the particle energy distributions, and (panel c) a zoomed-in view showing drift-kink driven deformations of the current sheet.

2 RESEARCH OBJECTIVES AND MILESTONES

The main goal of our one year campaign is to study the global plasma dynamics and local kinetics of pulsar magnetospheres to uncover fundamental processes that drive electromagnetic radiation. We will employ the well-established first-principles, relativistic, particle-in-cell method and use the exascale WarpX code to push the state-of-the-art towards realistic pulsar systems. With this one year proposal, our objective is to study the effect of scaling down the magnetic field strength and quantify the effect of injection rate on Poynting flux, dissipation rate, and particle acceleration for global pulsar simulations. We also will study the fundamental processes that accelerate particles in the magnetosphere We will use a dual-pronged approach to achieve this objective: (1) Use a wide computational lens to perform fully-kinetic, global, three-dimensional PIC simulations of pulsar magnetospheres and study the microscale mechanisms that affect the global spindown rate and Poynting flux of the system with scaled down magnetic field strength, (2) use focused ("zoomed-in") simulations to examine magnetic reconnection in the current sheet in order to quantify the energy transfer from the electromagnetic fields to the thermal, and kinetic energy in the current sheet for high magnetization.

We will measure the progress of our strategy described above using the following milestones. The first two milestones are targeted towards the current sheet simulations, wherein, we will study the effect of domain-size (Milestone 1) and the effect of guide field (Milestone 2) on 3D reconnection features, such as, flux ropes evolution and growth rate of tearing-mode and drift kink instability. In milestones 3 and 4, we will perform global pulsar magnetosphere simulations and study the effect of scaling-down the magnetic field strength to reduce the difference in length-scales in first-principles simulations, and rate of plasma injection on macroscale properties, such as, Poynting flux, spin-down rate, and energy dissipation.

Descriptions of each milestone follow below, and the summary Milestone Table is Tab. 5.

2.1 Milestone 1 : Effect of domain size and resolution on tearing mode and drift kink instability in 3D relativistic magnetic reconnection

2.1.1 *Pilot simulations of 3D relativistic reconnection*

We performed pilot 3D PSATD reconnection simulations at σ=30 for a domain size of $(2048\times256\times1024)\lambda_{\rm sd}$, which is 4× smaller in the y-direction than the proposed baseline 3D simulation (Tab. 1). We use Crusher, the 192-node testbed for the forthcoming Frontier system at OLCF. Our pilot simulations were 8-node Crusher runs, which are twice as coarse as our production runs in every dimension. Despite their smaller domain size and lower resolution, they demonstrate our ability to capture the basic structures expected of 3D magnetic reconnection: the tearing mode and drift-kink instabilities (panels (a) and (c) of Fig. 5), as well as some particle acceleration (panel (b) of Fig. 5). We ran our pilot simulations until a physical time of 1.3×10^{-7} s, which is about two-thirds of the physical time for our production reconnection simulation. We also extended this problem to develop a weak scaling test for Crusher, extending from 1 node up to 128 nodes. Further details of the weak scaling study can be found in Sec. 3.3.1 and Fig. 7.

2.1.2 *Proposed 3D relativistic reconnection simulations*

Due to the computational expense, and availability of resources, 3D magnetic reconnection studies (representative of realistic high energy plasma environments) are under-explored compared to their 2D counterparts. We will perform a first of its kind production-size 3D relativistic magnetic reconnection simulation using the ultra-high order PSATD solver. Our proposed baseline simulation will have magnetization σ = 30, resolution $dx = dy = dz = \lambda_{\rm sd}/2$, and domain-size $(2048\times1024\times1024)\lambda_{\rm sd}$. We will quantitatively compare the energy-transfer from fields to particles, power-law spectra, and reconnection rate, following the diagnostics we have developed for 2D reconnection (see section 3.2.3 and figure 6) [20]. We will also perform simulations with varying out-of-plane domain length (0.5× and 2× our fiducial $L_y = 1024\lambda_{\rm sd}$). This is a particularly interesting dimension to explore, since the evolution of the drift-kink instability and flux-rope structures develop along this direction, and can exhibit strong stochastic variability [36]. We will also verify convergence with a simulation using a higher spatial resolution. In both resolution and domain size studies, we will quantitatively compare the particle acceleration and evolution of the tearing mode and drift-kink instabilities to our baseline simulation. In total we will perform four relativistic simulations in this milestone to further understand the 3D physics of reconnection and study the effect of domain-size and resolution on the reconnection rate and particle acceleration.

We will run all four proposed simulations in this Milestone for three Alfven speed crossing times $3L_x/v_a$=0.208 μs, at which point reconnection will have saturated, and particle acceleration will be complete. The total walltime is estimated from the total number of PSATD timesteps required to complete the simulation and the walltime per timestep for each of these simulations. The walltime per timestep is obtained from a combination of coarser pilot simulations (Sec. 2.1.1) and their corresponding weak scaling performance (Sec. 3.3.1), which is described in detail in Sec. 3.1.4. Next, we estimated the number of GPU nodes that is necessary for our simulation. From our pilot 3D simulations and weak scaling studies (Sec. 2.1.1 and

Table 1. Summary of 3D relativistic reconnection simulations to study effect of domain size and resolution for Milestone 1*. Tab. 5 summarizes all milestones.

Case	Physical domain size $[L_x, L_y, L_z]\lambda_{\rm sd}$ $L_x = 2048$ $L_y =$ below $L_z = 1024$	Grid size $[n_x, n_y, n_z]$	Particles per cell $(e^+ + e^-)$	Physical time step (10^{-11} s)	Number of Frontier GPU nodes[a]	Total Wall-time (hrs)	Total node hours[b]
Baseline	1024	[4096, 2048, 2048]	54	1.65	256	14.4	3,700
$0.5L_y$	512	[4096, 1024, 2048]	54	1.65	128	14.4	1,900
$2L_y$	2048	[4096, 4096, 2048]	54	1.65	512	14.4	7,400
2x res	1024	[8192, 4096, 4096]	16	0.83	607	2.88	17,500
Total Node hours (NH) for Milestone 1 simulations							**30,500**

* Simulation parameters for all runs in this table : v_a/c=0.95; Physical simulation time $3L_x/v_a = 0.208$ μs
Walltime per timestep is 4.1 s, as estimated from pilot 3D simulations and weak scaling studies (see discussion in section 3.1.4).
[a] The box size for all the simulations in the milestone is $128 \times 128 \times 128$. All simulations but high resolution on the last row use 4 Boxes/GPU. Last row uses on average 13.5 boxes/GPU (i.e. half of GPUs will be initialized with 13, and half with 14; despite the initial imbalance, the computational load will become even as the simulation progresses, see load balancing discussion in Sec. 3.3.2)
[b] Node hour counts are rounded up to the nearest factor of 100

Sec. 3.3.1), we find that four 128^3 boxes with 54 particles per cell can saturate the GPU memory, allowing enough space for dynamic load balancing. We keep this computational load consistent throughout our $dx = dy = dz = \lambda_{\rm sd}/2$ simulations (first four rows of Tab. 1). As a result, the number of Frontier GPU nodes required per simulation changes depending on the size of our domain, and, in turn, grid. When we explore higher spatial resolution, we keep the number of particles per physical volume approximately constant, and aim to keep a comparable computational load per GPU. We can achieve this by allocating (on average) 13.5 128^3 boxes per GPU, with 16 particles per cell. While the computational load per GPU will initially be unbalanced, the computational load per box will shift throughout the simulation, allowing our load balancing algorithm (see Sec. 3.3.2) to evenly distribute the workload. The details of the domain size, grid size, particles per cell, walltime per timestep, number of Frontier nodes, walltime, and corresponding node hours required for all the simulations proposed in this Milestone is given in Tab. 1.

In summary, for Milestone 1, we will perform four 3D reconnection simulations with $\sigma = 30$ using the ultra-high order PSATD method, requiring 30,500 node hours. The results obtained from the simulations will be used to study the rich reconnection physics in 3D with detailed analysis of field to particle energy transfer. In particular, we will examine the effect of box size along the direction of the drift-kink instability on the development and growth rate of this instability. The studies will also inform us about the degree of convergence we achieve with our chosen resolution.

2.2 Milestone 2 : Effect of guide field on 3D relativistic reconnection

2.2.1 Proposed 3D relativistic reconnection simulations with guide fields

Studies have shown that for a magnetization of $\sigma = 10$, the guide field stabilizes the drift-kink instability [7, 11, 35]. However, the effect of guide field on tearing mode and drift-kink instability and how it affects the field to particle energy transfer and how different are they for relativistic reconnection is under explored. We will perform simulations to study the effect of the guide field for highly relativistic $\sigma = 30$ reconnection, by varying the $\alpha_g = 0.25, 0.5, 1$, where, α_g is the ratio of the guide-field to the in-plane magnetic field strength. We will quantitatively compare the particle energy spectra from these simulations using methods similar to those used to make Fig. 5 and also study the changes to reconnection rate and development of tearing mode and drift kink instabilities. These simulations will enable us to understand how the field energy is converted to heating versus non-thermal particle acceleration and how the guide field affects these quantities in the relativistic regime. Some of the diagnostics required to perform these analysis are discussed in Sec. 3.2.3. Similar to the simulations proposed in Milestone 1, we will dynamically load balance the simulations using Morton Z-ordered curves (Sec. 3.3.2).

Table 2. Summary of 3D reconnection simulations to study effect of Guide Field*. A summary of all milestones can be found in Tab. 5.

σ	$\alpha_g = \frac{B_g}{B_o}$	v_a/c	Physical simulation time = $3L_x/v_a$ (μs)	Number of timesteps	Number of Frontier GPU nodes	Total Walltime (hrs)	Total Node hours[a]
30	0.25	0.955	0.214	13,000	256	4.71	3,800
30	0.50	0.883	0.232	14,100	256	5.10	4,200
30	1.00	0.701	0.292	17,700	256	6.42	5,200
Total Node hours (NH) for Milestone 2 simulations							**13,200**

* Simulation parameters for all runs in this table : Physical domain size $L_x \times L_y \times L_z = (2048 \times 1024 \times 1024)\lambda_{\rm sd}$;
Particles per cell ($e^+ + e^-$): 54; Walltime per timestep = 4.1 s; Physical timestep = 1.65×10^{-11} s. Grid size ($n_x \times n_y \times n_z$) = $4096 \times 2048 \times 2048$; Box-size $128 \times 128 \times 128$, Boxes/GPU : 4
[a] Node hour counts are rounded up to the nearest factor of 100

We will perform three $\sigma = 30$ simulations with varying guide field strength. All simulations proposed for Milestone 2 will be performed for a domain size of $(2048 \times 1024 \times 1024)\lambda_{\rm sd}$, with $dx = dy = dz = \lambda_{\rm sd}/2$, initialized with 54 particles per cell and for 3 Alfven crossing times[27], matching our baseline 3D simulation. The inertial guide field will reduce the effective Alfven speed, $v_a = c\sqrt{\sigma/(1+\sigma(1+\alpha_g^2))}$[27], thereby requiring longer simulation times with increasing α_g. The timestep, Δt, for all simulations is 1.65×10^{-11} s, and the walltime per timestep for these 256-node Frontier simulations is estimated to be 4.1 s, as in Milestone 1 (see Sec. 2.1). The addition of a guide field does not affect the walltime per timestep. The numerical parameters required to perform these simulations and the corresponding number of Frontier GPU nodes, walltime, and node hours are given in Tab. 2.

In Milestone 2, we will quantitatively compare the effect of guide field on particle energization (heating versus acceleration) for 3D relativistic reconnection. To achieve this Milestone, we will perform three 3D reconnection simulations, requiring a total of 13,200 node hours.

2.3 Milestone 3 : Effect of scaling on electromagnetic energy dissipation and Poynting flux for millisecond pulsars

Milestones 1 and 2 will enable us to understand the fundamental processes that drive particle acceleration in current-sheets. We now describe simulations to zoom-out and study the global pulsar magnetosphere structure and emission sites. The difference in length-scale between the smallest skin-depth, $\lambda_{\rm sd}$ that would need to be resolved is at-least orders of magnitude smaller than the pulsar radius, R^*, which subsequently is smaller than the light-cylinder radius, R_{LC}. Capturing all the length scale-differences with a fully-kinetic PIC simulation is computationally intractable. This makes it necessary to scale-down the magnetic-field strength of the system while maintaining the same hierarchy of length-scales, $\lambda_{\rm sd} << R^* < R_{LC}$. Therefore, we are proposing to study the effect of scaling down $R^*/\lambda_{\rm sd}$ by performing simulations at varying values of scaling. Towards this effort, we have performed precursor simulations to demonstrate the capability of our code to perform these simulations, as shall be discussed next.

2.3.1 *Precursor scaled-down global pulsar magnetosphere simulations*

We performed pilot 3D pulsar magnetosphere simulations using PSATD for a scaled-down system with $R^*/\lambda_{\rm sd} = 6$, and a grid size of $768 \times 768 \times 768$, which is approximately 8-9 cells per skin-depth. Similar to the plasma injection method discussed in Brambilla et al.[5], we inject plasma-pair in the cells at the pulsar surface, to achieve a prescribed rate f, if the local plasma magnetization, $\sigma_M > \Sigma(\frac{R^*}{r})^3$[25, 5, 19], where, $\sigma_M = \frac{B_o^2}{\mu_0(n_e+n_i)m_e c^2}$ and Σ_o is the magnetization of the pulsar at the magnetic poles, B_o is the magnetic field strength, n_e, n_i are electron and ion number density, m_e is electron mass, and c is the speed of light. The rate of injection is defined as $f * F_{GJ}$, where $F_{GJ} = \frac{2\rho_{GJ}c}{q_e}$[5] is the Goldreich-Julian flux, ρ_{GJ} is the Goldreich-Julian charge density, c is the speed of light, q_e is the elementary charge, and the factor of 2 is for the two magnetic poles1.1. Similar to the simulations we propose in Milestone 4, we performed simulations to study effect of rate of injection on the plasma structure in the magnetosphere, as shown in Figs. 1-4. This demonstrates our capability of performing proposed simulations at scale with pair-plasma injected at a specified rate and an active equatorial current-sheet. Note that, the boundary condition on the surface is imposed using a stair-cased approximation in our simulations due to the use of a Cartesian grid. In order to accurately represent the spherical boundary, we required at-least 256 cells in each direction. Hence, for simulations with a large skin-depth, instead of using 3 cells per skin-depth which would be too coarse, we propose to use a minimum grid-size of 512^3 to resolve the spherical pulsar surface using the Cartesian grid.

The same set-up with same computational load per GPU as proposed in the Milestones 3 and 4 was also used to perform weak-scaling studies discussed in Sec. 3.3.1. These simulations were also used to estimate the walltime per timestep for the proposed 3D global pulsar magnetosphere simulations to be performed on the upcoming Frontier system (discussed in detail in Sec. 3.1.4). We also compared PSATD simulations with FDTD and found that the results are not different for the same resolution. But, the time required to complete 1000 timesteps for a grid size of $(512 \times 512 \times 512)$ with 2 GPU nodes on Crusher is 985 and 695 s for PSATD and FDTD Yee-solver, respectively. Although, PSATD is 1.4 times slower than the Yee method, the timestep allowed for the same CFL is 1.73 times larger in PSATD and Yee. Thus, PSATD completed 1.11 pulsar rotations in 1000 timesteps for the scaled-down tests used for the weak-scaling tests, while FDTD completed only 0.64 rotations. As a result, in terms of evolution of physical time, PSATD and Yee walltimes are comparable, while PSATD employs an ultra-high order solver compared to the second order Yee scheme. We now discuss the simulations proposed to study the effect of scaling down the magnetic field strength in the global pulsar magnetosphere simulations.

2.3.2 *Proposed 3D studies to study effect of $\frac{R^*}{\lambda_{sd}}$ scaling*

Although scaled-down simulations are considered a norm for pulsar PIC simulations, a detailed analysis of the effect of scaling on the simulation is still not available. Thus, in this milestone, we will study the effect of scaling down $R^*/\lambda_{\rm sd}$ by varying the scaling from 10, 25, 50, 100, 200, and 400, as listed in Tab. 3, with a resolution of 1 cell per skin-depth, using the ultra-high order PSATD solver. The largest simulation has a scaling of 400, which has not been analysed in 3D for a millisecond pulsar with an obliquity of 45 and proposed high resolution of 1cell/skin-depth (i.e., grid size of $(4800 \times 4800 \times 4800)$). Previous studies with 3D pulsar systems either used a smaller scaling or coarsened the resolution by not resolving the skin-depth within the light-cylinder radius[19], which caused artificial numerical heating. Note that the baseline test used to compare the scaling effect has 100 scaling with 1 cell/skindepth (row 2 in Tab. 3).. This resolution is the highest that we have found in the literature, for this scaling in 3D systems. We also study boundary effects by increasing the domain-size from $(4 \times 4 \times 4)R_{LC}$ to $(6 \times 6 \times 6)R_{LC}$. All the simulations are performed with an injection rate of $5F_{GJ}$, for 4 rotations by which time, the plasma reaches steady-state. Wwe use 3 cells/skin-depth for the baseline pulsar simulation (row 1 in Tab. 3), to especially compare the effect of different injection rates proposed in Milestone 4. However, for all the scaling runs, we choose a resolution of 1 cell/skin-depth to compare the results, keeping the resolution the same.

Table 3. Summary of 3D pulsar magnetosphere simulations to study effect of scaling and verify convergence. Tab. 5 summarizes all milestones.

scaling = $\frac{R^*}{\lambda_{sd}}$	Physical Domain-size L * R_{LC}	Grid size $n_x = n_y = n_z$	Number of cells per λ_{sd}	Number of timesteps	No. of Frontier GPU nodes	Total Walltime (hrs)	Total Node hours (rounded)[a]
100 (injection baseline)	[4,4,4]	4,800	3	30,500	1,648	15.25	25,200
100 (scaling baseline)	[4,4,4]	1,600	1	10,500	62	5.25	400
100 (larger domain)	[6,6,6]	2,400	1	10,500	206	5.25	1,100
10	[4,4,4]	160	1	1000	1	1.75	2
10	[4,4,4]	512	3	2500	2	1.75	4
25	[4,4,4]	512	1	2500	2	1.75	4
50	[4,4,4]	800	1	4000	8	3.0	30
200	[4,4,4]	3,200	1	15,500	489	10.25	5,100
400	[4,4,4]	6,400	1	35,500	3,907	20.25	79,200
Total Node hours (NH) for Milestone 3 simulations							**111,040**

[*] Simulation parameters for all runs in this table : Light Cylinder Radius $R_{LC} = 48,000$ m;
Pulsar Radius = 12,000 m, Injection Rate = 5 F_{GJ} ; Particles per cell ($e^+ + e^-$): 50; Walltime per timestep = 1.8 s; cfl = 0.99; All simulations are performed for 4 rotations. Box-size $64 \times 64 \times 64$, Boxes/GPU : 32
[a] Node hour counts for jobs > 100 NH are rounded up to the nearest factor of 100

The timing estimates for the proposed 3D pulsar simulations proposed in this milestone were carefully calculated from a combination of coarser pilot simulations (Sec. 2.3.1) and the corresponding weak scaling performance (Sec. 3.3.1). We extrapolated the weak scaling performance for the high GPU nodes as required for the proposed simulations to be walltime per timestep of 1.8 s, for each PSATD simulation, discussed in Sec. 3.1.4. The details of total number of nodes, node hours, wall time, simulations parameters for this Milestone are given in Tab. 3. In order to extract the Poynting flux, energy dissipation, and spin-down rate, we will use an in-situ reduced-diagnostic capability in WarpX, which is discussed further in Sec. 3.2.3. The analysis and diagnostic capability incorporated in Milestones 1 and 2 for the 3D reconnection studies will be used again to study the energy transfer from the fields to the particles in the equatorial current sheet.

For Milestone 3, we will perform we will perform eight 3D simulations with varying R^*/λ_{sd} scaling, using the ultra-high order PSATD method, requiring 111,040 node hours (breakdown in Tab. 3). We will use the simulations to study the effect of scaling down the magnetic field strength on the structure and composition of the magnetosphere, and on quantities such as the Poynting flux and spin down rate.

2.4 Milestone 4 : Effect of injection rate on the magnetosphere structure and Poynting Flux

Proposed 3D global pulsar magnetosphere simulations for Milestone 4

Pulsars are known to operate between two regimes: a vacuum magnetosphere with low density plasma and the force-free magnetosphere with highly dense plasma. Previous works have modeled pair-production by injecting plasma at a desired rate enabling the study of different pulsar configurations. However, the effect of plasma injection on the 3D plasma structure and particle acceleration sites of millisecond pulsars with a scaling ration of 100 are still under explored. We will perform simulations to study various configurations of millisecond pulsars, in a spectrum of charge-separated electrospheres to dense magnetospheres by varying

Table 4. Summary of 3D pulsar magnetosphere simulations to study effect of injection rate (F). A summary of all milestones can be found in Tab. 5.

F	$scaling = \frac{R^*}{\lambda_{sd}}$	Grid-size $n_x = n_y = n_z$	No. of cells per λ_{sd}	Number of timesteps	No. of Frontier GPU nodes	Total Walltime (hrs)	Total Node hours[a]
0.2	100	4,800	3	30,500	1,648	15.25	25,200
0.5	100	4,800	3	30,500	1,648	15.25	25,200
1.0	100	4,800	3	30,500	1,648	15.25	25,200
10.0	100	4,800	3	30,500	1,648	15.25	25,200
Total Node hours (NH) for Milestone 4 simulations							**100,800**

* Simulation parameters for all runs in this table : Physical domain size $L_x \times L_y \times L_z = (4 \times 4 \times 4)R_{LC}$; Particles per cell ($e^+ + e^-$): 50; Walltime per timestep = 1.8 s; Box-size $64 \times 64 \times 64$, Boxes/GPU : 32
[a] Node hour counts are rounded up to the nearest factor of 100

the injection rate, $f = 0.2, 0.5, 1.0, 5.0, 10.0$[19, 5].

All simulations for this Milestone will be performed for 4 pulsar rotations (30,500 timesteps), with a domain size of (4×4×4)R_{LC}, resolution with 3 cells/λ_{sd} ($dx = dy = dz$ =40 m) resulting in a grid-size of (4800×4800×4800). The obliquity for all simulations in this Milestone is $\chi = 45$ and timestep, Δt, is 1.32×10^{-7} s. The walltime per timestep required for these simulations, performed using 1,648 Frontier GPU nodes, is estimated to take an average of 1.8 s which includes the time required for dynamic load balancing, diagnostics, and checkpointing/restart (Sec. 3.1.4). The numerical parameters required to perform these simulations and the corresponding number of Summit GPU nodes, walltime, and node hours are given in Tab. 4. We will also perform detailed analysis on the trajectory of particles and analyse which regions in the magnetosphere form primary acceleration sites for 3D oblique pulsar magnetospheres.

In summary, from our final Milestone, we will be able to quantitatively compare the effect of plasma injection rate on energy dissipation, total electromagnetic field energy, and particle energization for 3D global pulsar magnetosphere simulations. To achieve this Milestone, we will perform four 3D global pulsar simulations which will require a total of 100,800 node hours.

3 COMPUTATIONAL READINESS

WarpX[32, 22] is highly optimized to run efficiently on leadership class facilities and employs customized data-structures for grid attributes, parallelization, dynamic load balancing, communication strategies, and GPU-offloading provided by the AMReX software [37, 38]. Both WarpX and AMReX are developed under the Exascale Computing Project (ECP), and open-source for use by a larger community via Github. Even though WarpX is primarily developed for modeling plasma wakefield particle accelerator devices, the advanced numerical algorithms for modeling high-energy relativistic plasma can also be leveraged for modeling particle acceleration in astrophysical processes. Any improvements contributed to the code through the work proposed, such as, algorithmic and diagnostics enhancements, will thus benefit our collaboration as well as the larger astro-plasma community.

3.1 Use of Resources Requested

3.1.1 Preparation for the MI250X AMD GPUs

Although AMReX, which provides the underlying framework for WarpX, provides the backend necessary to perform simulations on NVIDIA, Intel, and AMD GPUs, a few changes were required specific to the PIC method as it uses a lot of atomic operations. These operations are proportional to the number of particles, which are on the order of 500 billion particles. We thus performed a careful analysis of the atomic operations on Crusher using our pilot tests. When compiling for AMD MI250X GPUs, i.e., gfx90a target, the Clang compiler provides a flag '-munsafe-fp-atomics' which can suggest to the compiler to use hardware floating point atomic operations. The flag is however (prior to ROCm 5.2.0), only a *suggestion* to the compiler, which means compiling with the flag is not a binding agreement that the hardware atomic will be used. This can, potentially, have severe consequences for performance (which we have verified in tests not presented here), as software (i.e. compare-and-swap) implementations of the atomic operations require many more cycles to complete than their counterpart hardware atomics. ROCm exposes (prior to ROCm 5.2.0) the hardware atomic add through a function 'unsafeAtomicAdd', which ensures the hardware atomic add (rather than the compare-and-swap) is used. Thus to ensure optimum performance of the WarpX's CurrentDeposition kernel, we use the hardware atomic with 'unsafeAtomicAdd'. In forcing usage of the hardware atomic add, we are careful to guard against a known behavior wherein the hardware atomic can give incorrect results (which is the origin of the word 'unsafe' in the flags and function described above) when the hardware atomic acts on fine-grained memory allocations. This behavior is particularly insidious for memory allocated with 'hipMallocManaged', which returns a fine-grained memory allocation by default. So, to ensure performance and correctness, we force usage of the hardware atomic add, and accumulate into coarse-grained memory allocations in GPU global memory (which is the default memory returned with 'hipMalloc'). We found these changes made a significant difference of a factor of 10 to our walltime per timestep for the pilot simulations.

3.1.2 ***Description of the largest and longest runs***

As mentioned previously, most of the proposed simulations in Milestones 3 and 4 require more than 1,024 Frontier GPU nodes to perform the wide-lens global pulsar magnetosphere simulations. The largest pulsar simulation is for a scaling ratio 4× (row 9 of Tab. 3) that of the scaling baseline (row 2 of Tab. 3), requiring grid-size of 6400^3, and 3,907 GPU nodes on Frontier with a walltime of 20.25 hours to complete 4 pulsar rotations, resulting in 79,200 node hours. This is one of the largest scaling ratio performed for a well-resolved 3D simulation with pulsar obliquity of 45, grid-size 6400^3, and injection rate of $5F_{GJ}$ and is necessary to study the effect of the scaled-down magnetic field strength on the structure, composition, particle acceleration computed from simulations. The simulations in Milestone 4 require 1,648 nodes with a walltime of 15.25 hours to complete 4 pulsar rotations (30,500 timesteps) with a grid-size of $4{,}800^3$. For the simulations with more than 10 hours of walltime, we will use our checkpoint/restart capability implemented in WarpX and tested with our pilot 3D simulations to ensure continuity of simulations.

3.1.3 ***Burn rate of the allocation***

We split our allocation usage over the 1 year campaign such that, for the first four months of our proposed work, we will perform the zoomed-in relativistic magnetic reconnection simulations proposed in Milestones 1 and 2 using 43,700 node hours, that is nearly 17% of our total request. We will then increase our burn rate due to the aforementioned large and long runs in Milestones 3 and 4, each requiring four months. By September 2023, we expect to have used upto 60% of the total requested time. The remaining 100,800 node hours will be used for Milestone 4.

3.1.4 ***Estimation of walltime per timestep for the proposed 3D reconnection and pulsar simulations***

For the relativistic reconnection simulations proposed in Milestones 1 and 2, weak scaling tests on Crusher and Summit indicate that our largest runs (600 nodes) should have a weak scaling efficiency of greater than 80%, and that correspondingly, the walltime per timestep in our largest reconnection runs is likely less than or equal to 3.3 s, not including load-balancing or I/O. Additional tests with I/O and load balancing increased the walltime per timestep by 25%. This results in a total time per timestep estimate of 4.1 s for our production reconnection simulations. Since the weak scaling behavior is approximately flat, we use 4.1 s as our estimated time per timestep in all of our 3D reconnection runs tabulated in Tab. 1 and 2 for Milestones 1 and 2, respectively.

For the proposed global pulsar magnetosphere simulations in Milestones 3 and 4, the average workload is 4 boxes of size 128^3 per GPU. We performed pilot simulations and weak scaling tests on the Crusher test-bed (discussed in Sec. 3.3.1) which showed that the walltime per GPU is nearly 1.1 s per timestep with load-balancing and without I/O. We also performed additional tests with I/O required to analyze the results (including reduced diagnostics discussed in Sec. 3.2.3) which showed that the walltime per timestep increases by 25%. With the near-ideal scaling efficiency on Crusher and nearly 80% scaling efficiency on Summit, we estimated a conservative walltime per timestep as 1.8 s for the global pulsar magnetosphere simulations proposed for Milestones 3 and 4, as also mentioned in Tab. 3 and 4, respectively.

3.1.5 Data management : short and long term storage

Our estimate for storage requirements are based on data generated for analysis, visualization, and diagnostics and checkpoint, which will be used to restart our simulations. Majority of the reconnection simulations listed in Milestones 1 and 2 will generate plotfiles with particles and field data of size upto 5 TB. However, the largest reconnection simulation (row 4 of Tab. 1) will require 43 TB for the full plotfile data. Similarly, the largest pulsar magnetosphere simulations proposed in Milestones 3 (rows 1 and 9 in Tab. 3) require about 43 and 83 TB for the full plotfile output and all simulations in Milestone 4 require 35 TB. To save memory footprint, we will only generate them every 1000-2000 timesteps and instead generate slice data every 100 timesteps for more fine-grained analysis. The estimated size of the slice data is 150 GB for the largest pulsar magnetosphere simulation, and the total slice data generated is equal to the size of two full plotfiles. We will also generate reduced diagnostics (discussed in Sec. 3.2.3) every 20 timesteps. This capability is a special feature in WarpX which allows for a reduced memory footprint (0.002 GB size) and yet enables us to extract the necessary data, such as panel (b) of Fig. 5. From these files, we estimate that simulations proposed in Milestone 1 and 2 will require 200-400 TB of short term storage.

In comparison, the large pulsar simulations proposed in Milestones 3 and 4 will require 3-5 PB of short term storage. Our analysis will also generate smaller files, such as, particle histograms and distribution functions, field and particle energy data at shorter time intervals, leading to less than 24 GB of data for each simulation. This data will allow us to study power law scaling and quantify how much field energy is converted to particle heating and non-thermal acceleration. For longer Milestones 3 and 4 with walltimes (>10 hours), a checkpoint file will be generated every 5 hours (every 10,000 timesteps) from the start of the simulation. On average, each checkpoint file for the largest Milestone 3 simulation (row 9 of Tab. 3) is 2 PB, as it this simulation includes 16 trillion particles and 262 billion cells. The Orion filesystem to be deployed on Frontier for I/O includes a hard-disk-based capacity tier that provides 679 PB capacity, enabling us to perform these large-scale simulations. When a new checkpoint file is generated, the previous checkpoint file will be deleted to ensure that there is enough space on scratch to perform these runs.

We request long term storage to keep a copy the reduced data-set, coarsened slice data and few coarsened full snapshots generated for all the simulations, which sums up to less than 1 PB for each milestone, and a grand total of 2.2 PB. A breakdown of the short and long term storage for each milestone is given in the Milestone Table (Tab. 5) at the end of the document. We will use Globus to transfer data from Frontier to the long-term HPSS file storage and expect to need these for atleast six months after the end of the INCITE allocation cycle for further analysis towards our future publications.

3.1.6 Leadership Classification

We have previously demonstrated excellent scaling on the Summit machine as part of the ECP WarpX project[22]. To demonstrate readiness of our application on Frontier, we have also demonstrated good weak scaling performance for the proposed magnetic reconnection and pulsar magnetosphere simulations on Crusher, discussed in Sec. 3.3. Leaving some buffer memory required for load balancing and particle redistribution, we can saturate the memory on a single MI250x AMD GPU using four boxes of size 128^3 with 54 particles per cell. The physics of 3D reconnection and pulsar magnetosphere requires us to use larger domain with higher resolution leading to grid sizes of upto 6400^3 necessitating just shy of 4,000 GPU nodes on Frontier (32,000 MI250X AMD GPUs). Our largest reconnection simulation will have 137 billion grid cells at 2.2 trillion particles and the global pulsar magnetosphere simulations proposed in Milestones 3 and 4 will have 110 billion cells and nearly 7 trillion particles. The large amount of particle and field data generated will also require between 1–5 PB of short term scratch space, and approximately 2 PB of long term storage. This is only possible with access to leadership class facilities.

We request a total of 255,540 NH with 4.9 and 2.2 PB of short- and long-term storage, In order to support open science and data reproducibility, the simulation input files, code versions, derived results, and scripts will be published on a data archive such as Zenodo.org. We will submit our findings, made possible through the INCITE program, to peer-reviewed journals.

3.2 Computational Approach

In the electromagnetic (EM) PIC approach, charged plasma species are modeled as computational particles, each representing a large number of real ions and electrons, and the EM fields are evolved on the grid. A typical PIC timestep involves particle-to-grid deposition of charge density, ρ, and current density, J, that are used to self-consistently compute the time-dependent EM fields by solving Maxwell's equations. Finally, the EM forces are interpolated from the grid to particles which are accelerated to new positions using Newton's laws and leap-frogging scheme. Most of the advanced PIC codes used for astrophysical plasma simulations employ the finite difference time domain (FDTD) approach to solve Maxwell's equation. While WarpX includes traditional explicit FDTD algorithms, it also has an option of higher-order pseudo-spectral analytic time-domain (PSATD) solver[31, 14] that suppresses numerical dispersion which the FDTD counterparts experience. From our pilot simulations, we found that for the same problem size, FDTD and PSATD produce similar results, however, the PSATD simulations were faster in terms of walltime required per physical time.

WarpX is written to C++17 standards and employs an MPI+X paradigm, where the backend support for GPUs is provided by AMReX. WarpX is well tested for plasma wakefield accelerators and many of the features required also apply to the proposed relativistic astrophysical plasma simulations. Additionally, to enable pulsar magnetosphere simulations, we have added modules in the code to apply boundary conditions on the pulsar surface and plasma injection algorithm.[5]. Additional astro-plasma specific capability, such as the implementation of Maxwell-Juttner distribution, particle tagging diagnostics, momentum averaging, and reduced-diagnostic capabilities added to WarpX, as part of this project, will also be made open-source on github to benefit the collaboration with WarpX, as well as the larger plasma simulation community.

3.2.1 I/O Requirements

In the proposed WarpX simulations, I/O consists of checkpoint files for restart capability and plotfiles for visualization. We will use the asynchronous I/O functionality in AMReX to write plotfiles to disk in a non-blocking fashion. Furthermore, we will utilize scalable I/O capabilities of WarpX with both openPMD and plotfile capability that interface to ADIOS1, ADIOS2, and HDF5. For analysis and visualization of simulations proposed in this work, we will especially take advantage of the reduced in-situ diagnostics[12] to compute particle energy spectra for reconnection and Poynting flux, dissipation, magnetic energy density, and electromagnetic energy density for pulsar magnetospheres. More such reduced diagnostics are actively being pursued in WarpX to significantly reduce the memory footprint of our results. Tape storage will be required to archive and compare simulation snapshots over the runtime of the campaign, as discussed in Sec. 3.1.5. Note that this is only for analysis purposes; our simulations themselves will not access tape storage.

3.2.2 Libraries, Programming Languages

To compile and execute our code, we need a C++17 compiler compatible with the available CUDA/NVCC version, CMake 3.22.1 or newer, and for Frontier AMD GPUs, we use HIP provided by the ROCM compiler stack. We used the craype-accel-amd-gfx90a environment to perform the pilot simulations on Crusher. For

PSATD runs, we will need FFTW-3 and cuFFT libraries. We will need ADIOS1 and ADIOS2 with MPI support, ASCENT for in-situ visualization, and openPMD-api, python, and yt for analysis of our results.

3.2.3 *Analysis, Software Workflow, and IO requirements*

Our simulation analysis consists of in situ WarpX diagnostics and Python-based post-processing, where we use numpy, h5py, matplotlib, mpi4py, and yt. We also use Jupyter notebooks with parallel, multi-node and GPU support provided by OLCF resources. Through the ECP project, we have implemented interfaces for in-situ visualization using ASCENT, and can use VisIt and ParaView to inspect the large 3D plotfiles our simulations will output. We will use WarpX's diagnostics framework to output full plotfiles containing information about the fields as well as custom diagnostics such as average particle velocity. This has been particularly valuable in yielding measurements of the spatial variation in inflow and exhaust velocity at the X-points which we use to calculate the rate of reconnection for our 2D simulations [20]. An example plot created for this analysis is shown in Fig. 6. We will apply this same analysis to slices from the proposed 3D simulations. We also use the reduced diagnostics to calculate particle energy histograms on the fly, like the one shown in panel (b) of Fig. 5. We have a pipeline to calculate the fastest-growing Fourier modes in the x, y, and z directions, and we can compare this analysis to theoretical expectations, e.g. [9]. Similar to the reconnection simulation, we will use averaged particle velocities to investigate plasma trajectories along the current sheet and also study the particle power spectra. The same reduced diagnostic capabilities will be used to compute the dissipation, Poynting flux, and electromagnetic energy density at various radii from the pulsar surface.

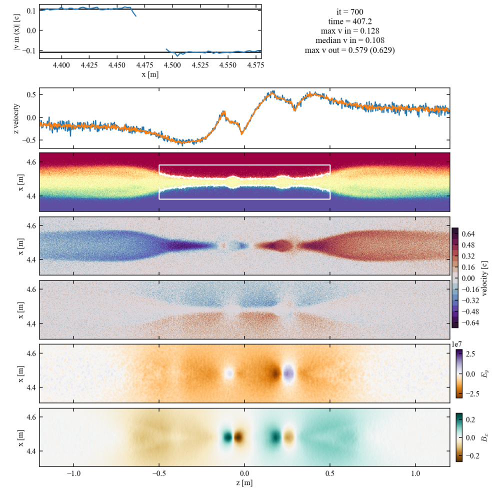

Figure 6. Example diagnostic panel for our 2D reconnection simulations [20], similar to those we will make for slices of our 3D simulations. From top to bottom, we show average inflow velocity profile, average outflow velocity profile, mixing between plasma above and below current sheet, outflow velocity, inflow velocity, reconnection electric field E_y, and x-component of the magnetic field B_x.

3.3 Parallel Performance

3.3.1 *Weak Scaling*

The weak-scaling performance is most relevant to our large-scale simulation estimates, as it keeps the computational load per GPU the same across different simulations, while increasing the problem size proportionally. In this section, we will describe the weak scaling studies that we performed on the 192-node Crusher testbed, using pilot 3D simulations for magnetic reconnection and global pulsar magnetospheres, previously described in Secs. 2.1.1 and 2.3.1, respectively. Additionally, we show weak scaling performance on Summit to demonstrate our capability to perform the proposed production runs on more than 1000 GPU nodes on Frontier.

Relativistic Magnetic Reconnection Weak Scaling : We studied the weak-scaling behavior of the reconnection simulation on Crusher from 1-128 nodes using the PSATD solver. We used four 128^3 boxes per GPU and 54 particles per cell, representative of the production simulations proposed for Milestones 1 and 2. The scaling runs were performed for 200 timesteps and did not include I/O or load balancing. From pilot simulations we know that the walltime per timestep is relatively constant throughout the simulation with dynamic load balancing, so this early period is representative of the whole evolution. We find that the time per timestep is approximately 2.6 s from 1 to 128 nodes (see fig. 7). We demonstrate our ability to scale to > 128 nodes with similar weak scaling tests on Summit, where we see > 80% scaling efficiency between 1 and 512 nodes. Given that Crusher outperforms Summit on weak scaling efficiency from 1 to 128 nodes, we expect that Crusher's scaling efficiency will be better than 80% even for our largest reconnection simulations (607 nodes).

Global Pulsar Magnetosphere Weak Scaling: We also performed weak-scaling studies of the pulsar magnetosphere simulations on Crusher using the PSATD solver. For these simulations, we used an average of 4 boxes of size 128^3 per GPU, representative of the pulsar magnetosphere simulations proposed in Milestones 3 and 4. We found that this problem size with nearly 50 particles per species leaves sufficient GPU memory for dynamic load balancing, particle redistribution, and communication. As is typical for weak scaling studies, we kept the computational load per GPU constant and increased the number of GPUs proportional to the problem size, from 512^3 grid on 2 Crusher GPU nodes to a grid size of 2048^3 for 128 Crusher nodes. We ran our tests for 1,000 timesteps, enough to complete nearly 1 rotation, and found that our walltime per timestep is 1.1 s on 2 Crusher nodes, and remains nearly constant with increase in the number of GPU nodes on Crusher (shown in Fig. 8), indicating near-ideal efficiency. Since Crusher has 192-nodes, we also performed weak scaling on Summit with a smaller workload per GPU. From Fig. 8, it can be seen that the walltime per timestep on Summit for a work load of 8 boxes/GPU with box size 128^3 is 0.92 s per timestep, and increases by 13% to 1.04 s per timestep on 512 nodes. The walltime per timestep is smaller on Summit due to the reduced workload per GPU compared to the tests performed on Crusher, however, similar to the reconnection test, the efficiency on Crusher outperforms that on Summit. Thus we expect the efficiency to remain > 80% resulting in a walltime per timestep of 1.8 s even for our largest pulsar simulation, that is performed with 3,907 Frontier GPU nodes.

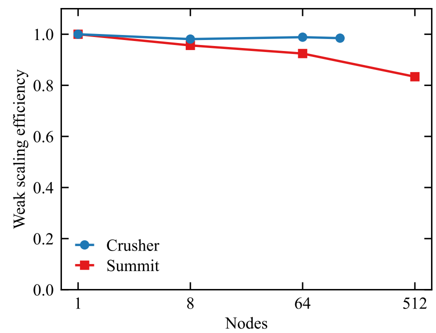

Figure 7. Weak scaling efficiency of 3D reconnection simulations on Crusher (blue) and Summit (red), used to estimate walltime for MS 1&2 in Sec. 3.1.4.

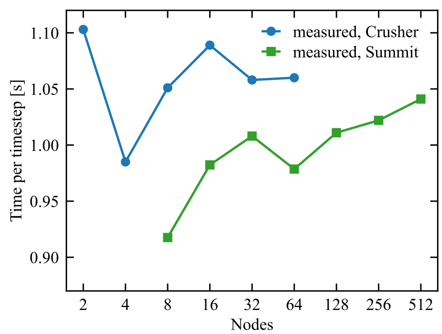

Figure 8. Weak scaling efficiency of 3D pulsar simulations on Crusher (blue) and Summit (green) is > 85% and used to estimate WallTime per timestep in Sec. 3.1.4.

3.3.2 *Dynamic Load Balancing*

In both the reconnection and pulsar simulations, the plasma particles are not evenly distributed between the computational subgrids. Without load balancing, we are likely to overload a few GPUs while leaving others idle and therefore, load balancing is essential in our simulation for efficient use of Frontier resources. To adapt to the time-varying computational expense of different parts of the domain, the *distribution mapping*, i.e. mapping from boxes in the physical domain to MPI ranks is updated on-the-fly, also known as *dynamic* load balancing. Further details of our in-situ cost measurement strategies on GPUs and load balancing algorithms are provided in Ref. [26]. WarpX has multiple algorithmic options for determining a distribution mapping. The two main options are a) Knapsack method that randomly distributes subgrids to GPUs and b) Z-ordered space filling curve (SFC) method, which keeps physically adjacent subgrids on the same GPU. We found that for reconnection and pulsar magnetosphere simulations, the SFC mapping yields a lower walltime per timestep than the Knapsack distribution by 20% due to data locality and optimized particle communication patterns. We will therefore use dynamic load balancing with a SFC distribution mapping in all of our production runs.

3.4 Developmental Work

We are ready to perform production simulations and the corresponding data analysis as soon as INCITE allocations start in January 2023. All of the necessary functionality described in this proposal has been implemented and tested in mainline WarpX and/or our reconnection- and pulsar-specific forks. Independent of the proposed work, WarpX and AMReX are continuously being enhanced and optimized for leadership-class supercomputers. These improvements are not essential for the success of our work, but allow us to quickly take advantage of new features in the software environment.

References

[1] AA Abdo, Markus Ackermann, Marco Ajello, A Allafort, Luca Baldini, Jean Ballet, Guido Barbiellini, D Bastieri, K Bechtol, R Bellazzini, et al. Gamma-ray flares from the crab nebula. *Science*, 331(6018):739–742, 2011.

[2] Ester Aliu, T Arlen, T Aune, M Beilicke, W Benbow, A Bouvier, SM Bradbury, JH Buckley, V Bugaev, K Byrum, et al. Detection of pulsed gamma rays above 100 gev from the crab pulsar. *Science*, 334(6052):69–72, 2011.

[3] M Balbo, R Walter, C Ferrigno, and P Bordas. Twelve-hour spikes from the crab pevatron. *Astronomy & Astrophysics*, 527:L4, 2011.

[4] G. Blaclard, H. Vincenti, R. Lehe, and J.L. Vay. Pseudospectral Maxwell solvers for an accurate modeling of Doppler harmonic generation on plasma mirrors with particle-in-cell codes. *Physical Review E*, 96(3), 2017.

[5] Gabriele Brambilla, Constantinos Kalapotharakos, Andrey N Timokhin, Alice K Harding, and Demosthenes Kazanas. Electron–positron pair flow and current composition in the pulsar magnetosphere. *The Astrophysical Journal*, 858(2):81, 2018.

[6] Benoît Cerutti, Alexander Philippov, Kyle Parfrey, and Anatoly Spitkovsky. Particle acceleration in axisymmetric pulsar current sheets. *Monthly Notices of the Royal Astronomical Society*, 448(1):606–619, March 2015.

[7] Benoit Cerutti, Gregory R Werner, Dmitri A Uzdensky, and Mitchell C Begelman. Three-dimensional relativistic pair plasma reconnection with radiative feedback in the crab nebula. *The Astrophysical Journal*, 782(2):104, 2014.

[8] Alexander Y Chen and Andrei M Beloborodov. Electrodynamics of axisymmetric pulsar magnetosphere with electron-positron discharge: a numerical experiment. *The Astrophysical Journal Letters*, 795(1):L22, 2014.

[9] L. Comisso, M. Lingam, Y. M. Huang, and A. Bhattacharjee. Plasmoid Instability in Forming Current Sheets. *The Astrophysical Journal*, 850(2):142, December 2017.

[10] Contopoulos, I. The role of reconnection in the pulsar magnetosphere. *A&A*, 466(1):301–307, 2007.

[11] J. T. Dahlin, J. F. Drake, and M. Swisdak. The mechanisms of electron heating and acceleration during magnetic reconnection. *Physics of Plasmas*, 21(9):092304, September 2014.

[12] WarpX development team. Warpx documentation. https://warpx.readthedocs.io/en/latest/.

[13] CB Forest, K Flanagan, M Brookhart, M Clark, CM Cooper, V Désangles, J Egedal, D Endrizzi, IV Khalzov, H Li, et al. The wisconsin plasma astrophysics laboratory. *Journal of Plasma Physics*, 81(5), 2015.

[14] Brendan B Godfrey, Jean-Luc Vay, and Irving Haber. Numerical stability analysis of the pseudo-spectral analytical time-domain pic algorithm. *Journal of Computational Physics*, 258:689–704, 2014.

[15] Fan Guo, Yi-Hsin Liu, William Daughton, and Hui Li. Particle Acceleration and Plasma Dynamics during Magnetic Reconnection in the Magnetically Dominated Regime. *The Astrophysical Journal*, 806(2):167, June 2015.

[16] Revathi Jambunathan, Hannah Klion, Michael Rowan, Andrew Myers, Jean-Luc Vay, and Weiqun Zhang. Effect of particle injection rate on 3d pulsar simulations. *Manuscript in preparation*.

[17] Hantao Ji, Amitava Bhattacharjee, Stewart Prager, W Daughton, Stuart D Bale, T Carter, Neal Crocker, J Drake, Jan Egedal, John Sarff, et al. Flare (facility for laboratory reconnection experiments): a major next-step for laboratory studies of magnetic reconnection. *AAS/AGU Triennial Earth-Sun Summit*, 1:104–05, 2015.

[18] Hantao Ji, William Daughton, Jonathan Jara-Almonte, Ari Le, Adam Stanier, and Jongsoo Yoo. Magnetic reconnection in the era of exascale computing and multiscale experiments. *Nature Reviews Physics*, pages 1–20, 2022.

[19] Constantinos Kalapotharakos, Gabriele Brambilla, Andrey Timokhin, Alice K Harding, and Demosthenes Kazanas. Three-dimensional kinetic pulsar magnetosphere models: connecting to gamma-ray observations. *The Astrophysical Journal*, 857(1):44, 2018.

[20] Hannah Klion, Revathi Jambunathan, Michael Rowan, Andrew Myers, Jean-Luc Vay, and Weiqun Zhang. Simulations of relativistic magnetic reconnection using pseudo-spectral methods. *Manuscript in preparation*.

[21] F Curtis Michel and Hui Li. Electrodynamics of neutron stars. *Physics reports*, 318(6):227–297, 1999.

[22] A Myers, A Almgren, LD Amorim, J Bell, L Fedeli, L Ge, Kevin Gott, David P Grote, M Hogan, Axel Huebl, et al. Porting warpx to gpu-accelerated platforms. *Parallel Computing*, 108:102833, 2021.

[23] Jérôme Pétri. Theory of pulsar magnetosphere and wind. *Journal of Plasma Physics*, 82(5), 2016.

[24] Alexander A Philippov and Anatoly Spitkovsky. Ab initio pulsar magnetosphere: three-dimensional particle-in-cell simulations of axisymmetric pulsars. *The Astrophysical Journal Letters*, 785(2):L33, 2014.

[25] Alexander A. Philippov, Anatoly Spitkovsky, and Benoit Cerutti. Ab Initio Pulsar Magnetosphere: Three-dimensional Particle-in-cell Simulations of Oblique Pulsars. *The Astrophysical Journal Letters*, 801(1):L19, March 2015.

[26] ME Rowan, A Huebl, KN Gott, J Deslippe, M Thévenet, R. Lehe, and J-L Vay. In-situ assessment of device-side compute work for dynamic load balancing in a gpu-accelerated pic code. In *Proceedings of the Platform for Advanced Scientific Computing Conference (PASC '21)*, 2021.

[27] Michael Rowan. *Dissipation of Magnetic Energy in Collisionless Accretion Flows*. PhD thesis, Harvard University, 2019.

[28] Lorenzo Sironi and Anatoly Spitkovsky. Relativistic reconnection : An efficient source of non-thermal particles. *The Astrophysical Journal*, 783(1):L21, feb 2014.

[29] Allen Taflove and Susan C Hagness. *Computational electrodynamics*, volume 28. Artech house publishers Norwood, MA, 2000.

[30] Dmitri A. Uzdensky and Anatoly Spitkovsky. PHYSICAL CONDITIONS IN THE RECONNECTION LAYER IN PULSAR MAGNETOSPHERES. *The Astrophysical Journal*, 780(1):3, dec 2013.

[31] J.-L. Vay, I. Haber, and B.B. Godfrey. A domain decomposition method for pseudo-spectral electromagnetic simulations of plasmas. *Journal of Computational Physics*, 243:260–268, 2013.

[32] Jean-Luc Vay, Ann Almgren, John Bell, Guillaume Blaclard, Lixin Ge, Dave Grote, Mark Hogan, Haithem Kallala, Remi Lehe, Andrew Myers, et al. Warp-x: a new exascale computing platform for plasma simulations. In *APS Division of Plasma Physics Meeting Abstracts*, volume 2018, pages TO8–004, 2018.

[33] H. Vincenti and J.-L. Vay. Ultrahigh-order Maxwell solver with extreme scalability for electromagnetic PIC simulations of plasmas. *Computer Physics Communications*, 2018.

[34] Stodiek von Goeler, W Stodiek, and N Sauthoff. Studies of internal disruptions and m= 1 oscillations in tokamak discharges with soft—x-ray tecniques. *Physical Review Letters*, 33(20):1201, 1974.

[35] Gregory R. Werner and Dmitri A. Uzdensky. Nonthermal Particle Acceleration in 3D Relativistic Magnetic Reconnection in Pair Plasma. *The Astrophysical Journal*, 843(2):L27, 2017.

[36] Gregory R. Werner and Dmitri A. Uzdensky. Reconnection and particle acceleration in three-dimensional current sheet evolution in moderately magnetized astrophysical pair plasma. *Journal of Plasma Physics*, 87(6):905870613, December 2021.

[37] Weiqun Zhang, Ann Almgren, Vince Beckner, John Bell, Johannes Blaschke, Cy Chan, Marcus Day, Brian Friesen, Kevin Gott, Daniel Graves, et al. Amrex: a framework for block-structured adaptive mesh refinement. *Journal of Open Source Software*, 4(37):1370–1370, 2019.

[38] Weiqun Zhang, Andrew Myers, Kevin Gott, Ann Almgren, and John Bell. Amrex: Block-structured adaptive mesh refinement for multiphysics applications. *International Journal of High Performance Computing Applications*, 2021.

PERSONNEL JUSTIFICATION AND MANAGEMENT PLAN

PERSONNEL JUSTIFICATION

Personnel on this proposal represent core-developers, designers, and architects of the main simulation code, WarpX, as well as the AMReX software framework. In addition to the personnel listed below, a number of collaborators on the Exascale Computing Project working on WarpX will support the development of WarpX for the laser-plasma accelerations which are synergistic with this application.

- **Revathi Jambunathan** is an early-career Research Scientist in the Center for Computational Sciences and Engineering (CCSE) at LBNL and will serve as the lead for this project. She will run the proposed global pulsar magnetosphere simulations along with Hannah and contribute to the code-development as needed for this project. She contributes to the ECP-funded WarpX code and also is a core-developer and maintainer of the ARTEMIS code for modeling electromagnetic signals in ARTEMIS.
- **Hannah Klion** is a postdoctoral scholar in the CCSE at LBNL. Her expertise lies in computational astrophysics and she contributes to WarpX code. She will run the proposed simulations along with the lead PI and perform detailed analysis extracting meaningful physical insight from the simulations and disseminating them into publications.
- **Michael Rowan** is a MTS Software Development Engineer at AMD. His expertise lies in computational plasma physics using PIC methods applied to relativistic magnetic reconnection, and he was the lead architect of dynamic load balancing in AMReX, that we heavily leverage in WarpX for the proposed simulations. Michael will contribute to both the analysis of magnetic reconnection to extract important physical details and also guide us with optimizations for AMD GPUs.
- **Andrew Myers** is a Computer Systems Engineer in CCSE at LBNL. His work centers on implementing and optimizing algorithms for particle methods in AMReX and WarpX, HPC programming, as well as scientific visualization. From the time of its inception, Andrew also contributes to the science and algorithm development in WarpX for pulsar magnetosphere simulations.
- **Jean-Luc Vay** is the PI of the ECP-project for modeling advanced plasma accelerators using WarpX. He is also the main architect of the advanced numerical algorithms for relativistic plasma physics that is implemented in WarpX. Jean-Luc Vay will guide the choice of algorithms for energy and momentum conservation, FDTD, PSATD, and other advanced hybrid algorithms for our proposed simulations.
- **Weiqun Zhang** is a Computer Systems Engineer in CCSE at LBNL. He is the lead-architect of the AMReX framework used in WarpX. He will especially contribute to the optimization revolving mesh-refinement in WarpX that is critical component of the proposed project.

MANAGEMENT PLAN

The researchers on this proposal are part of CCSE and ATAP at LBNL and and also from AMD. We collaborate on the ECP-projects, WarpX and AMReX, and the team has a proven track record of developing optimized GPU-accelerated code, and performing large-scale simulations for plasma acceleration on Summit as well as other computing resources. The team-members are funded for code-development work via Department of Energy's Exascale Computing Project, "Advanced Accelerator Modeling Program" and "Block-Structured AMR Co-Design Center". There is no subdivision of time for sub-teams. Our expertise and skills are complementary, and we will employ a unified approach to carry out the milestones described in the proposal. Simulation decisions for this campaign are proposed by the PI with advice from M.Rowan, H.Klion, A.Myers, and J.L.Vay. The simulations will be performed by the lead PI and Co-PI, H.Klion who will also perform detailed analysis of the simulations. The Co-PIs H.Klion, M.Rowan, and A.Myers, will also provide their expertise on PIC simulations for astrophysical plasma and scientific insights on relativistic reconnection (expertise from M. Rowan) and astrophysical environment of compact objects (A. Myers and H.Klion). For this project, J.L.Vay will provide his expertise on computational plasma physics, especially for relativistic plasma, numerical algorithms for energy and momentum conservation, and higher-order spectral methods. W.Zhang is a core-developer and designer of the AMReX code, and his skills are invaluable to the parallelization, communication, and load balancing implementations required for the proposed simulations in this campaign. All the developmental work for modeling particle acceleration in astrophysical plasma are synergistic with that for the ECP-funded particle accelerator modeling project. Although, our roles may seem distinct, we will all be involved in the science analysis and the team-members will be co-authors on the publications that results from the proposed simulations.

Points of contact for updates on the status of the work including publications, awards, and highlights of accomplishments are Revathi Jambunathan rjambunathan@lbl.gov and Jean-Luc Vay jlvay@lbl.gov

4 Milestone Table

Milestone Table

Milestone	Details	Dates
Milestone 1 Effect of domain size and resolution on tearing mode and drift kink instability in 3D relativistic magnetic reconnection	**Resources:** Frontier **Node hours:** 30,500 NH **Filesystem storage (TB and dates):** upto 727 TB by end of February, 2023 **Archival storage (TB and dates) :** upto 380 TB of reduced diagnostics, slices, and full plotfiles will be stored in HPSS by end of March, 2023 **Software Application:** WarpX **Tasks:** Perform four 3D magnetic reconnection simulations with σ=30 using 128–607 Frontier GPU nodes. Quantify how domain size and resolution affect the reconnection rate, development of tearing mode and drift-kink instability, and particle acceleration. Simulation parameters with walltime, GPU nodes, and node hours are summarized in Tab. 1. **Dependencies:** None	February 2023 (expected)
Milestone 2 Effect of guide field on 3D relativistic reconnection	**Resources:** Frontier **Node hours:** 13,200 NH **Filesystem storage (TB and dates):** upto 270 TB by end of April, 2023 **Archival storage (TB and dates):** 153 TB of reduced diagnostics, slices, and relevant full plotfiles will be stored in HPSS by the end of May 2023 **Software Application:** WarpX **Tasks:** Perform three 3D magnetic reconnection simulations with different values of guide field, drawn from values expected in the current sheets that surround pulsars. Quantify how guide field affects the rate of reconnection, the evolution of tearing mode and drift-kink instabilities, and the non-thermal particle acceleration. Simulation parameters with walltime, GPU nodes, and node hours are summarized in Tab. 2. **Dependencies:** None	April 2023 (expected)
Milestone 3 Effect of scaling on electromagnetic energy dissipation and Poynting flux for millisecond pulsars	**Resources:** Frontier **Node hours:** 111,040 NH **Filesystem storage (TB and dates):** upto 4.9 PB by end of August 2023 **Archival storage (TB and dates):** upto 660 TB of reduced diagnostics, slices, and relevant full plotfiles should be saved to HPSS by the end of September 2023 **Software Application:** WarpX **Tasks:** Perform six global pulsar magnetosphere simulations with varying R^*/λ_{sd} scaling using 1 cell per skin-depth to study the effect of scaling down the magnetic field strength on the computed Poynting flux. Perform a simulation with R^*/λ_{sd} with 3 cells/skin-depth to study convergence and also perform convergence studies with a larger domain size. Simulation parameters for all the proposed runs with walltime, GPU nodes, and node hours are summarized in Tab. 3. **Dependencies:** None	August 2023 (expected)
Milestone 4 Effect of injection rate on the magnetosphere structure and Poynting Flux	**Resources:** Frontier **Node hours:** 100,800 NH **Filesystem storage (TB and dates):** upto 2.9 PB by end of December 2023 **Archival storage (TB and dates):** upto 970 TB of reduced diagnostics, slices, and relevant full plotfiles should be saved by end of December 2023 **Software Application:** WarpX **Tasks:** Perform four global pulsar magnetosphere simulations with R^*/λ_{sd}=100 and varying plasma injection rate to study the effect of injection rate of magnetosphere structure, particle acceleration, and Poynting flux. Simulation parameters with walltime, GPU nodes, and node hours are summarized in Tab. 4 **Dependencies:** None	December 2023

PUBLICATIONS RESULTING FROM PREVIOUS INCITE AWARDS

New award proposal; no previous publications.

Curriculum Vitae
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Professional Preparation

PhD, Department of Aerospace Engineering, University of Illinois, Urbana-Champaign, May 2019
MS, Department of Aerospace Engineering, University of Illinois, Urbana-Champaign, December 2012
BS, Aeronautical Engineering, Nehru College of Aeronautics and Applied Sciences, India, 2008

Appointments

2021–present - Research Scientist career-track, Center for Computational Sciences and Engineering, LBNL

2019–2021 - Postdoctoral Researcher, Center for Computational Sciences and Engineering, LBNL

2013–2019 - Graduate Research Assistant, Department of Aerospace Engineering, University of Illinois, Urbana-Champaign.

2010–2012 - Teaching Assistant, Electrical and Computer Engineering, University of Illinois, Urbana-Champaign.

2008-2010 - Assistant Research Engineer, Compressor Division, Gas Turbine Research Establishment, Bangalore, India

Five Publications Most Relevant to This Proposal

1. R Jambunathan, H Klion, A Myers, M Rowan, J.L.Vay and W.Zhang, *"Effect of Particle Injection Rate on 3D Pulsar Simulations"*, *In-preparation*
2. H Klion, R Jambunathan, M Rowan, A Myers, J.L.Vay and W.Zhang, *"Simulations of Relativistic Magnetic Reconnection using Pseudo-Spectral Methods"*, *In-preparation*
3. R Lehe, A Belly, L Giacomel, R Jambunathan *"Absorption of charged particles in Perfectly-Matched-Layers by optimal damping of the deposited current"*, *submitted to Physical Review Letters E*
4. A Myers, A Almgren, L D Amorim, J Bell, L Fedeli, L Ge, K Gott, D P Grote, M Hogan, A Huebl, R Jambunathan, R Lehe, C Ng, M Rowan, O Shapoval, M Thévenet, J.-L Vay, H Vincenti, E Yang, N Zaïm, W Zhang, Y Zhao, E Zoni, *"Porting WarpX to GPU-accelerated platforms"*, *Parallel Computing*
5. J.-L. Vay, A. Huebl, A. Almgren, L. D. Amorim, J. Bell, L. Fedeli, L. Ge, K. Gott, D. P. Grote, M. Hogan, R. Jambunathan, R. Lehe, A. Myers, C. Ng, M. Rowan, O. Shapoval, M. Thevenet, H. Vincenti, E. Yang, N. Zaïm, W. Zhang, Y. Zhao, and E. Zoni, *"Modeling of a chain of three plasma accelerator stages with the WarpX electromagnetic PIC code on GPUs"*, Phys. Plasmas 28, 023105 (2021) *Special Collection: Building the Bridge to Exascale Computing: Applications and Opportunities for Plasma Science*

Research Interests and Expertise

I am interested in developing GPU-optimized electrodynamics codes for modeling astrophysical plasma processes, particle-accelerators, and next-generation microelectronics. I am specifically interested in leveraging mesh-refinement for bridging scale-disparity in physical systems and exploring hybrid continuum-kinetic approaches.

Synergistic Activities

1. Co-PI on an Berkeley lab LDRD proposal (2022-2023)
2. Organized and chaired mini-symposium "Kinetic Simulations of Astrophysical Processes" at SIAM CSE conference, 2021.
3. Peer-Reviewer for CAMCoS, CPC
4. Reviewer for Small Business Innovation Research (SBIR) proposals, 2020.
5. Application track committee member for the 49th International Conference on Parallel Programming (ICPP), 2020.
6. Contributor to ECP-project, WarpX, (J-L. Vay, PI) WarpX
7. Developer and maintainer of electrodynamics code, ARTEMIS

Collaborators (*past 5 years including name and current institution*)

Ann Almgren (Lawrence Berkeley National Laboratory)
Diana Amorim (Lawrence Berkeley National Laboratory)
John Bell (Lawrence Berkeley National Laboratory)
Lixin Ge (SLAC National Accelerator Laboratory)
Kevin Gott (Lawrence Berkeley National Laboratory)
David Grote (Lawrence Livermore National Laboratory)
Axel Huebl (Lawrence Berkeley National Laboratory)
Michael Rowan (Lawrence Berkeley National Laboratory)
Remi Lehe (Lawrence Berkeley National Laboratory)
Andrew Myers (Lawrence Berkeley National Laboratory)
Don Willcox (Lawrence Berkeley National Laboratory)
Cho Ng (SLAC National Accelerator Laboratory)
Andrew Nonaka (Lawrence Berkeley National Laboratory)
Zhi (Jackie) Yao (Lawrence Berkeley National Laboratory)
Olga Shapoval (Lawrence Berkeley National Laboratory)
Maxence Thevenet (DESY, Germany)
Jean-Luc Vay (Lawrence Berkeley National Laboratory)
Eloise Yang (Lawrence Berkeley National Laboratory)
Weiqun Zhang (Lawrence Berkeley National Laboratory)
Yinjian Zhao (Lawrence Berkeley National Laboratory)
Edoardo Zoni (Lawrence Berkeley National Laboratory)
Luca Fedeli (CEA, Saclay)
Neïl Zaïm, (CEA, Saclay)
Antoine Sainte-Marie, (CEA Saclay),
Henri Vincenti
Lorenzo Giacomel (CERN, Switzerland)

Hannah Klion
Lawrence Berkeley National Laboratory
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Professional Preparation

PhD in Physics, University of California, Berkeley (2021)
MA in Physics, University of California, Berkeley (2017)
BS in Physics (minor in Computer Science), California Institute of Technology (2015)

Appointments

2021–present - Postdoctoral Researcher, Center for Computational Science and Engineering, LBNL
2020–2021 - Graduate Student Researcher, Astronomy Department, University of California, Berkeley
2019–2020 - Physics Theory Graduate Fellow, University of California, Berkeley
2019 - Teaching Assistant, Astronomy Department, University of California, Berkeley
2015–2019 - Department of Energy Computational Science Graduate Fellow, University of California, Berkeley

Five Publications Most Relevant to This Proposal

1. R Jambunathan, **H Klion**, A Myers, M Rowan, J.L.Vay and W.Zhang, *Effect of Particle Injection Rate on 3D Pulsar Simulations*, *In-preparation*
2. **H Klion**, R Jambunathan, M Rowan, A Myers, J.L.Vay and W.Zhang, *Simulations of Relativistic Magnetic Reconnection using Pseudo-Spectral Methods*, *In-preparation*
3. **H. Klion**, A. Tchekhovskoy, D. Kasen, A. Kathirgamaraju, E. Quataert, R. Fernández (2022) *The impact of r-process heating on the dynamics of neutron star merger accretion disc winds and their electromagnetic radiation.* Monthly Notices of the Royal Astronomical Society, Volume 510, Issue 2, p. 2968.
4. **H. Klion**, P. Duffell, D. Kasen, E. Quataert (2021) *The Effects of Jet-Ejecta Interaction on 2D Kilonova Light Curves.* Monthly Notices of the Royal Astronomical Society, Volume 502, Issue 1, p. 865.
5. P. Duffell, E. Quataert, D. Kasen, **H. Klion** (2018) *Jet Dynamics in Compact Object Mergers: GW170817 Likely Had a Successful Jet.* The Astrophysical Journal, Volume 866, Issue 1, Article ID 3.

Research Interests and Expertise

High-performance multiphysics simulations, computational particle methods, magnetic reconnection, radiation transport, Monte Carlo methods, general relativistic hydrodynamics

Synergistic Activities

1. Selected as 2022 Rising Star in Computational and Data Sciences, Albuquerque, NM
2. Co-Investigator on 2022 ALCC Proposal (R. Jambunathan, PI)
3. Contributor to ECP-project, WarpX (J-L. Vay, PI)
4. Developer of Monte Carlo radiation transport code, Sedona (D. Kasen, PI)

Collaborators (*past 5 years including name and current institution*)

Ann Almgren (Lawrence Berkeley National Laboratory)
John Bell (Lawrence Berkeley National Laboratory)
Luca Fedeli (CEA, Saclay)
Lixin Ge (SLAC National Accelerator Laboratory)
Kevin Gott (Lawrence Berkeley National Laboratory)

David Grote (Lawrence Livermore National Laboratory)
Austin Harris (Oak Rdige National Laboratory)
Axel Huebl (Lawrence Berkeley National Laboratory)
Revathi Jambunathan (Lawrence Berkeley National Laboratory)
Dan Kasen (Lawrence Berkeley National Laboratory, Unviersity of California Berkeley)
Remi Lehe (Lawrence Berkeley National Laboratory)
Bronson Messer (Oak Ridge National Laboratory)
Andrew Myers (Lawrence Berkeley National Laboratory)
Cho Ng (SLAC National Accelerator Laboratory)
Eliot Quataert (Princeton University)
Michael Rowan (Lawrence Berkeley National Laboratory)
Olga Shapoval (Lawrence Berkeley National Laboratory)
Maxence Thevenet (DESY)
Jean-Luc Vay (Lawrence Berkeley National Laboratory)
Don Willcox (Lawrence Berkeley National Laboratory)
Weiqun Zhang (Lawrence Berkeley National Laboratory)
Yinjian Zhao (Lawrence Berkeley National Laboratory)
Edoardo Zoni (Lawrence Berkeley National Laboratory)

Curriculum Vitae: Andrew T Myers

Mail Stop 50A-3111, Lawrence Berkeley National Laboratory
Berkeley, CA 94720
atmyers@lbl.gov
510-387-6492

Professional Preparation

Ph.D. in Physics, University of California, Berkeley (2013)
B.S. in Physics, University of North Carolina, Chapel Hill (2006)

Appointments

1/2017 – present: Computer Systems Engineer, Center for Computational Sciences and Engineering (CCSE), Lawrence Berkeley National Laboratory.
10/2013 - 10/2016, Postdoctoral Researcher, Applied Numerical Algorithms Group, Lawrence Berkeley National Laboratory.

Five Publications Most Relevant to This Proposal

1. A Myers, A Almgren, L D Amorim, J Bell, L Fedeli, L Ge, K Gott, D P Grote, M Hogan, A Huebl, R Jambunathan, R Lehe, C Ng, M Rowan, O Shapoval, M Thévenet, J.-L Vay, H Vincenti, E Yang, N Zaïm, W Zhang, Y Zhao, E Zoni Porting WarpX to GPU-accelerated platforms, submitted to Parallel Computing
2. W Zhang, A Myers, K Gott, A Almgren, J Bell AMReX: Block-structured adaptive mesh refinement for multiphysics applications., The International Journal of High Performance Computing Applications. June 2021. doi:10.1177/10943420211022811
3. J-L Vay, A Almgren, J Bell, L Ge, DP Grote, M Hogan, O Kononenko, R Lehe, A Myers, C Ng, J Park, R Ryne, O Shapoval, M Thevenet, W Zhang, Warp-X: A new exascale computing platform for beam–plasma simulations, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 909, 476-479, 2018.
4. W Zhang, A Almgren, V Beckner, J Bell, J Blaschke, C Chan, M Day, B Friesen, K Gott, D Graves, Max Katz, A Myers, T Nguyen, A Nonaka, M Rosso, S Williams, M Zingale, (2019). AMReX: a framework for block-structured adaptive mesh refinement. Journal of Open Source Software, 4(37), 1370, https://doi.org/10.21105/joss.01370
5. A Myers, P Colella, B Van Straalen, A 4th-Order Particle-in-Cell Method with Phase-Space Remapping for the Vlasov-Poisson Equation, SIAM Journal on Scientific Computing 39(3), February 2016

Research Interests and Expertise I am a research software engineer and one of the developers of the AMReX library, where I focus on designing data structures and algorithms for implementing a variety of particle methods on current and upcoming supercomputing platforms. I'm especially interested in particle algorithms that interact with a block-structured adaptive mesh hierarchy. In addition to my work on AMReX, I also contribute to several ECP application projects, including the electromagnetic particle-in-cell code WarpX. I also have a background in astrophysics and experience developing tools for scientific data analysis and visualization.

Synergistic Activities

1. Member, Block-Structured AMR Co-Design Center (ECP)
2. Member, WarpX Project (ECP; J-L. Vay, PI)
3. Reviewer for Monthly Notices of the Royal Astronomical Society, Astrophysical Journal, Parallel Computing, and the International Journal of High Performance Computing Applications

Collaborators

Vincent Beckner (LBNL), John Bell (LBNL), Wes Bethel (LBNL), Johannes Blaschke (LBNL), David Camp (LBNL), Cy Chan (LBNL), Phillip Colella (LBNL) Marcus Day (LBNL), Anshu Dubey (ANL), Brian Friesen (LBNL), Lixin Ge (SLAC), Kevin Gott (LBNL), Daniel Graves (LBNL), David Grote (LLNL), Max Katz (NVIDIA), Richard Klein (LLNL), Remi Lehe (LBNL), Burlen Loring (LBNL), Chris McKee (UC-Berkeley), Andrew Nonaka (LBNL), Tan Nguyen (LBNL), Michele Rosso (LBNL), Brian Van Straalen (LBNL), Jean-Luc Vay (LBNL), Samuel Williams (LBNL), Weiqun Zhang (LBNL), Michael Zingale (SUNYSB)

Curriculum Vitae
MICHAEL E. ROWAN
mrowan137@gmail.com

Professional Preparation

Harvard University, Ph.D. in Physics (2013 – 2019)
Oberlin College, B.A.s in Physics and Mathematics (2009 – 2013)

Appointments

MTS Software Development Engineer, Advanced Micro Devices (2021–present)
NERSC Exascale Science Applications Postdoctoral Fellow, LBNL (2019–2021)

Five Publications Most Relevant to This Proposal

1. M.E. Rowan, A. Huebl, K.N. Gott, J. Deslippe, M. Thévenet, R. Lehe, & J.-L. Vay (2021). *In-situ Assessment of Device-side Compute Work for Dynamic Load Balancing in a GPU-accelerated PIC Code*. In Proceedings of the Platform for Advanced Scientific Computing Conference (PASC '21).
2. L. Sironi, M.E. Rowan, & R. Narayan (2021). *Reconnection-driven Particle Acceleration in Relativistic Shear Flows*. In ApJL 907 L44.
3. M.E. Rowan, L. Sironi, & R. Narayan (2019). *Electron and Proton Heating in Transrelativistic Guide Field Magnetic Reconnection*. In ApJ 873 1.
4. A. Chael, M.E. Rowan, R. Narayan, M.D. Johnson, & L. Sironi (2018). *The Role of Electron Heating Physics in Images and Variability of the Galactic Center Black Hole Sagittarius A**. In MNRAS 478 4.
5. M.E. Rowan, L. Sironi, & R. Narayan (2017). *Electron and Proton Heating in Trans-relativistic Magnetic Reconnection*. In ApJ 850 29.

Research Interests and Expertise Magnetic Reconnection, High-Performance Computing

Synergistic Activities

1. Co-organizer of GPU training event at LBNL: 'GPUs for Science 2020.'
2. Peer reviewer for CPC, PRE, PRX

Collaborators (*past 5 years including name and current institution*)

Ann Almgren (Lawrence Berkeley National Laboratory), Diana Amorim (Lawrence Berkeley National Laboratory), John Bell (Lawrence Berkeley National Laboratory), Wahid Bhimji (Lawrence Berkeley National Laboratory), Jack Deslippe (Lawrence Berkeley National Laboratory), Steve Farrell (Lawrence Berkeley National Laboratory), Lixin Ge (SLAC National Accelerator Laboratory), Kevin Gott (Lawrence Berkeley National Laboratory), David Grote (Lawrence Livermore National Laboratory), Mark Hogan (SLAC National Accelerator Laboratory), Axel Huebl (Lawrence Berkeley National Laboratory), Khaled Ibrahim (Lawrence Berkeley National Laboratory), Revathi Jambunathan (Lawrence Berkeley National Laboratory), Remi Lehe (Lawrence Berkeley National Laboratory), Andrew Myers (Lawrence Berkeley National Laboratory), Hai Ah Nam (Lawrence Berkeley National Laboratory), Cho Ng (SLAC National Accelerator Laboratory), Tan Nguyen (Lawrence Berkeley National Laboratory), Leonid Oliker (Lawrence Berkeley National Laboratory), Olga Shapoval (Lawrence Berkeley National Laboratory), Maxence Thevenet (DESY), Jean-Luc Vay (Lawrence Berkeley National Laboratory), Samuel Williams (Lawrence Berkeley National Laboratory), Nicholas Wright (Lawrence Berkeley National Laboratory), Eloise Yang (Lawrence Berkeley National Laboratory), Weiqun Zhang (Lawrence Berkeley National Laboratory), Yinjian Zhao (Lawrence Berkeley National Laboratory), Edoardo Zoni (Lawrence Berkeley National Laboratory), Ramesh Narayan (Harvard University), Lorenzo Sironi (Columbia University), Bob Bosch (Oberlin College), Jason Stalnaker (Oberlin College)

Curriculum Vitae
Dr. Jean-Luc Vay
jlvay@lbl.gov, 510-486-4934
ORCID: 0000-0002-0040-799X | Google Scholar Page
Lawrence Berkeley National Laboratory, ATAP Division
1 Cyclotron Road, M/S 71B-287, Berkeley, CA 94720, USA

Professional Preparation

PhD in Physics, University of Paris-Diderot, Paris, France. 1996
MS in Physics, University of Paris-Diderot, Paris, France. 1993
BS in Physics, University of Poitiers, Poitiers, France. 1991

Appointments

2013–now: Physicist Senior Scientist, Accelerator Technology & Applied Physics Division, LBNL
2005–2013: Physicist Staff Scientist, Accelerator & Fusion Research Division, LBNL
2000–2005: Physicist Scientist, Accelerator & Fusion Research Division, LBNL
1998–2000: Term Scientist, Accelerator & Fusion Research Division, LBNL
1996–1998: Postdoctoral Fellow, Accelerator & Fusion Research Division, LBNL

Five Publications Most Relevant to This Proposal

1. H. Vincenti, J.-L. Vay, "Ultrahigh-order Maxwell solver with extreme scalability for electromagnetic PIC simulations of plasmas", *Comput. Phys. Comm.* **228**, 22-29 (2018). https://doi.org/10.1016/j.cpc.2018.03.018
2. J.-L. Vay et al, "Warp-X: A new exascale computing platform for beam-plasma simulations", *Nucl. Inst. Meth. A* **909**, 486-479 (2018). https://doi.org/10.1016/j.nima.2018.01.035
3. J.-L. Vay, I. Haber, B. B. Godfrey, "A domain decomposition method for pseudo-spectral electromagnetic simulations of plasmas", *J. Comput. Phys.***243**, 260-268 (2013). https://doi.org/10.1016/j.jcp.2013.03.010
4. J.-L. Vay, D. P. Grote, R. H. Cohen, & A. Friedman, "Novel methods in the Particle-In-Cell accelerator code-framework Warp", *Computational Science & Discovery* **5**, 014019 (2012). http://dx.doi.org/10.1088/1749-4699/5/1/014019
5. J.-L. Vay, J.-C. Adam, A. Héron, "Asymmetric PML for the absorption of waves. Application to mesh refinement in electromagnetic particle-in-cell plasma simulations.", *Computer Physics Comm.*, **164**, 171-177 (2004). https://doi.org/10.1016/j.cpc.2004.06.026

Research Interests and Expertise

High-performance modeling of conventional - and advanced concepts - particle accelerators and light sources, for applications to discovery science, industry, security, energy, the environment and medicine. Advanced algorithms and parallel computing in application to large-scale simulations of charged particle beams, plasmas, accelerators and laser-plasma interactions.

Synergistic Activities

1. 2019: Theory and simulation group leader, Laser-Plasma Accelerator Workshop (LPAW19).
2. 2018: Chair of the APS DCOMP Nominating Committee.
3. 2016-present: PI DOE Exascale application project WarpX: Exascale modeling of advanced particle accelerators (also PI of NERSC, ALCF and OLCF repositories).
4. 2018-2021: PI INCITE project Plasm-In-Silico
5. 2016-2018: PI INCITE project PICSSAR
6. 2012-17: Co-PI of DOE Scientific Discovery through Advanced Computing SciDAC-ComPASS.
7. 2015-2020: PI NERSC repository for BELLA Center on modeling of advanced accelerators.

8. 2005-2016: PI of three and co-PI of two LDRD projects at LBNL.
9. 2015: Chair, WG on Theory and Simulations, European Advanced Accelerator Concepts Workshop (EAAC2015).
10. 2014: Chair, WG on Theory and Simulations, Advanced Accelerator Concepts Workshop (AAC2014).
11. 2014-2017: Member at large in exec. committee APS Division of Comput. Physics (DCOMP).
12. 2008-2014 Serving on the NERSC User Group Executive Committee NUGEX.
13. Fellow of the American Physical Society, Senior member of IEEE and member of the American Association for the Advancement of Science.

Collaborators (*past 5 years including name and current institution*) Ann Almgren, Lawrence Berkeley National Laboratory, USA
John Bell, Lawrence Berkeley National Laboratory, USA
Carlo Benedetti, Lawrence Berkeley National Laboratory, USA
David Bruhwiler, Radiasoft, USA
Stepan Bulanov, Lawrence Berkeley National Laboratory, USA
Nathan Cook, Radiasoft, USA
Eric Esarey, Lawrence Berkeley National Laboratory, USA
Alex Friedman, Lawrence Livermore National Laboratory, USA
Lixin Ge, Stanford Linear Accelerator Center National Laboratory, USA
Cameron Geddes, Lawrence Berkeley National Laboratory, USA
David Grote, Lawrence Livermore National Laboratory, USA
Axel Huebl, Lawrence Berkeley National Laboratory, USA
Haithem Kallala, CEA Saclay, France
Manuel Kirchen, University of Hamburg, Germany
Wim Leemans, DESY, Germany
Rémi Lehe, Lawrence Berkeley National Laboratory, USA
Burlen Loring, Lawrence Berkeley National Laboratory, USA
Andreas Maier, University of Hamburg, Germany
Cho Ng, Stanford Linear Accelerator Center National Laboratory, USA
Greg Penn, Lawrence Berkeley National Laboratory, USA
Oliver Ruebel, Lawrence Berkeley National Laboratory, USA
Robert Ryne, Lawrence Berkeley National Laboratory, USA
Olga Shapoval, Lawrence Berkeley National Laboratory, USA
Maxence Thévenet, Deutsches Elektronen-Synchrotron (DESY), USA
Carl Schroeder, Lawrence Berkeley National Laboratory, USA
Eric Stern, Fermilab National Accelerator Laboratory, USA
Frank Tsung, UCLA, USA
Henri Vincenti, CEA Saclay, France

Curriculum Vitae

Weiqun Zhang
Center for Computational Sciences and Engineering, Lawrence Berkeley National Laboratory
One Cyclotron Road, MS 50A-3111, Berkeley, CA 94720
email: weiqunzhang@lbl.gov

Professional Preparation

PhD in Astronomy and Astrophysics, University of California, Santa Cruz (2003)
BS in Plasma Physics, University of Science and Technology of China (1992)

Appointments

2013–present: Computer Systems Engineer, Lawrence Berkeley National Laboratory
2010–2013: Project Scientist, Lawrence Berkeley National Laboratory
2007–2010: Postdoc, New York University
2004–2007: Chandra Fellow, Stanford University
2003–2004: Postdoc, University of California, Santa Cruz

Five Publications Most Relevant to This Proposal

1. W. Zhang, A. Almgren, V. Beckner, J. Bell, J. Blaschke, C. Chan, M. Day, B. Friesen, K. Gott, D. Graves, M. Katz, A. Myers, T. Nguyen, A. Nonaka, M. Rosso, S. Williams, and M. Zingale, (2019). AMReX: a framework for block-structured adaptive mesh refinement. Journal of Open Source Software, 4(37), 1370, https://doi.org/10.21105/joss.01370
2. J.-L. Vay, A. Almgren, J. Bell, L. Ge, D.P. Grote, M. Hogan, O. Knonenko, R. Lehe, A. Myers, C. Ng, J. Park, R. Ryne, O. Shapoval, M. Thevenet, and W. Zhang, (2018). Warp-X: A New Exascale Computing Platform for Beam-Plasma Simulations. Nuclear Instruments and Methods in Physics Research Section A, 909, 476-479
3. M.N. Farooqi, T. Nguyen, W. Zhng, A.S. Almgren, J. Shalf, and D. Unat, (2018). Phase Asynchronous AMR Execution for Productive and Performant Astrophysical Flows. SC ’18 Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis, Article No. 70
4. Joseph D Gelfand, Patrick O Slane, and Weiqun Zhang, (2009). A dynamical model for the evolution of a pulsar wind nebula inside a nonradiative supernova remnant. ApJ, 703, 2051
5. Weiqun Zhang, Andrew MacFadyen, and Peng Wang, (2009). Three-dimensional relativistic magnetohydrodynamic simulations of the kelvin-helmholtz instability: Magnetic field amplification by a turbulent dynamo. ApJL, 692, L40

Research Interests and Expertise Astrophysical Flows, Radiation Transfer, Numerical Methods, High-Performance Computing

Synergistic Activities

1. Referee for various journals in astrophysics and high-performance computing (e.g., Astrophysical Journal, Astrophysical Journal Letters, and Parallel Computing).
2. Ph.D. thesis committee member, E. Lovegrove, UC Santa Cruz.
3. Mentor for GPU Hackathon
4. Mentor for US Department of Energy program: Science Undergraduate Laboratory Internships

Collaborators (*past 5 years including name and current institution*) Ann Almgren (LBNL), Vinamra Agrawal (Auburn University), Vincent Beckner (LBNL), John Bell (LBNL), Marcus Day (NREL), Matthew Emmett (Computer Modeling Group), M. N. Farooqi (Koc University), Kevin, Gott (LBNL), Ray Grout (NREL), Max Katz (Nvidia), Andrew Myers (LBNL), Michael Minnon (LBNL), Jordan Musser (NETL), Tan Nguyen (LBNL), Brandon Runnels (University of Colorado, Colorado Springs) John Shalf

(LBNL), Didem Unat (LBNL), Jean-Luc Vay (LBNL), Stanford Woosley (UCSC), Michael Zingale (Stony Brook)

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

WarpX (ECP-Project)

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

AMReX (ECP Project)

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

PICSAR

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

yt-project (visualization)

Indicate whether Open Source or Export Controlled.

Open Source

Package Name

Paraview (visualization)

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

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

Colleagues and collaborators, email notices, and OLCF websites, as well as LinkedIn/Twitter!

Question #2

Suggested Reviewers

Suggest names of individuals who would be particularly suited to assess the proposed research.

Dr. Amitava Bhattacharjee (amitava@pppl.gov)

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.

9_TestBed_INCITE23_RJ.pdf
The attachment is on the following page.

TestBed Resources

We do not anticipate requiring the testbed resources at ALCF and OLCF.