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3D modeling of the Staged Z-pinch with the FLASH code

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Abstract

The Staged Z-pinch (SZP) fusion concept is a magneto-inertial compression scheme developed by Magneto-Inertial Fusion Technologies, Inc. (MIFTI), in which small amounts of fusion fuel are brought to fusion-relevant conditions by passing multi-million amperes strong current through a cylindrical shell of high atomic number material. One- and two-dimensional modeling performed by MIFTI with the MACH2 code, suggests that net fusion energy gain can be achieved when currents in the 10 million amperes range compress a 50%-50% mixture of deuterium and tritium gas.

In this project we enhance and use the FLASH code to execute high-fidelity, simulations of various SZP configurations, a collaboration between the Flash Center for Computational Science at the University of Rochester and the Laboratory for Laser Energetics, and MIFTI. FLASH is a high-performance computing, multi-physics, radiation magnetohydrodynamic (MHD) code with extended physics capabilities, which is developed at the Flash Center. The goal of this project is to assess the shell/fuel stability of the pinch to two- and three-dimensional MHD instabilities and to utilize FLASH's extended physics capabilities to understand how extended-MHD effects impact implosion dynamics and plasma conditions at stagnation. The project is a natural extension of an ongoing collaborative effort between MIFTI and the Flash Center through the U.S. DOE Advanced Research Projects Agency-Energy (ARPA-E) BETHE program and can provide MIFTI with simulation capabilities that are currently beyond their reach with MACH2. Ultimately, MIFTI wants FLASH to become one of their simulation workhorses for reliable, high-fidelity SZP platform design.

During the project, the Flash Center team developed a suite of in one- and two-dimensional FLASH simulations to model different variants of the SZP platform, performed code-to-code comparisons with MACH2, and used the FLASH code to design and model SZP experiments like the Double Eagle experiments that MIFTI recently performed. Also, the Flash Center team developed the capabilities of FLASH to be able to do three-dimensional simulations of pulsed-power experiments with the code for the first time. Two publications from this effort are currently under review and two more are in preparation. MIFTI has also committed to the use of FLASH for future SZP simulation efforts.

1 Introduction and Scope

1.1 The Staged Z-pinch platform and Magneto-Inertial Fusion Technologies, Inc.

Scientists from the University of California, Irvine (UCI), and business professionals founded Magneto-Inertial Fusion Technologies, Inc. (MIFTI) in 2008. The company mission is to develop the so-called Staged Z-pinch concept as a clean fusion energy source. While several companies are pursuing different fusion ideas, few have experimentally achieved any significant thermonuclear neutron yield or shown a path to scalability. MIFTI's concept starts with the oldest fusion idea (the Z-pinch) and refines it by surrounding the fusion fuel with high atomic number cylindrical plasma shell. According to MIFTI, this shell provides several benefits which are discussed below.

While UCI scientists started exploring the Staged Z-pinch (SZP) both theoretically and experimentally more than 30 years ago, commercialization of the SZP concept was pursued by

MIFTI with the company formation and the filling of two patents: one for radionuclides and nuclear medicines production [1], and another for magneto-inertial fusion energy production [2]. A U.S. DOE ARPA-E ALPHA program award in 2015 provided significant impetus to MIFTI by making available funds for experiments on the 1 MA pulsed power generators Zebra (University of Nevada, Reno) and Cobra (Cornell University). The experiments on Zebra, with a krypton gas liner compressing a deuterium fuel, produced consistent thermonuclear fusion yield of up to 10^{10} neutrons, in good agreement with their MACH2 code calculations.

A Staged Z-pinch, shown in Figure 1, is a cylindrically symmetric multi-shell plasma column where the outer shell (i.e., the liner) is composed of high atomic number plasma and the inner plasma shell is composed of either DD or DT fusion fuel (i.e., the target). MACH2 calculations performed by MIFTI indicate that, with sufficiently large current drive, the platform may achieve fusion energy-relevant plasma temperature in the 10-20 keV range. In this concept, these temperatures are obtained by: (1) preheating the target plasma with inward propagating shock waves born in the liner, and (2) a very strong adiabatic compression of the target, close to the stagnation time, by a thin and very dense liner plasma layer. The shock strength depends on the Mach number $\mathrm{M} = \mathrm{v_r}/\mathrm{c_s}$, where $\mathrm{v_r}$ is the implosion velocity and $\mathrm{c_s} = \sqrt{\mathrm{T_e}/\mathrm{m_i}}$ is the sound speed. Higher atomic number liner plasmas have heaver ion mass $\mathrm{m_i}$ (i.e., lower sound speed), and thus can generate stronger shocks. They also radiate more and have a lower temperature, which facilitates the magnetic field diffusion, which contributes to the strength of magneto-sonic shocks. MACH2 calculations indicate that break-even, and beyond, fusion conditions are possible by applying a current $\geq$ 10 MA to a load made of Kr or Xe liner plasma and a DT target plasma. The concept was successfully tested two decades ago at UC Irvine, and most recently, during the ARPA-E ALPHA program on the 1 MA Zebra facility, and the 4 MA Double Eagle facility at L3Harris in San Leandro, California.

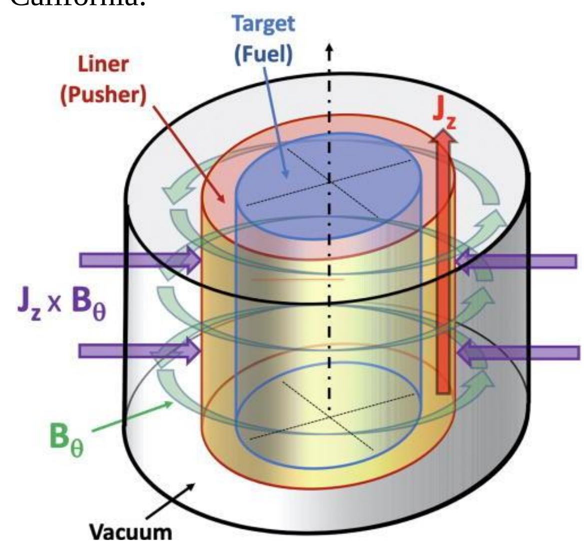

Figure 1. Schematic of a Staged Z-pinch [3]. The axial plasma current interacts with the self-generated azimuthal magnetic field B_θ and creates a $\boldsymbol{J} \times \boldsymbol{B}$ Lorentz force which compresses the column radially. In the final compression stage, the accumulated liner kinetic energy converts rapidly into target plasma thermal and radiation energy. With sufficiently intense final compression, target plasma conditions may satisfy the Lawson criterion $n_i T_i \tau_E > 3\times10^{21}$ keV s m^{-3}, thus producing net energy gain.

1.2 A simulation resource team for fusion concepts – ARPA-E BETHE

Modeling of high current Staged Z-pinches is of special interest because they provide large net fusion energy gain through alpha particle heating of the DT fusion fuel. In the past, MIFTI investigated several SZP configurations using the Sandia Z-pulsed power generator parameters [4-6], employing the MACH2 (Multi-block Arbitrary Coordinate Hydromagnetic 2) code [7]. MACH2 is a single-fluid, multi-material, three-temperature resistive MHD code, developed by the Center for Plasma Theory and Computation at the Air Force Research Laboratory (AFRL), Phillips Research Site. While MACH2 simulations have been successfully applied in a series of experiments, performed by MIFTI and their collaborators, all models of SZP to date have been limited to one- or two-dimensional MACH2 simulations, with limited extended-MHD effects. To explore the pinch's stability to current driven modes [8,9] like the kink, as well to account for multi-spatial effects in the magneto Rayleigh Taylor instability MRTI [10], full three-dimensional simulations are required, which allow for motions that traverse the symmetry axis of the pinch. Z-pinch variants that incorporate an axial magnetic field for stabilization have been shown [11] to be unstable to a helical instability, which again can only be captured by 3D simulations. Further, there are several regimes where resistivity, finite ion Larmor radius effects and other physics omitted in ideal MHD are important [12] and thermoelectric effects, such as the Nernst effect, can play a significant role in the transport of magnetic and thermal fluxes in magnetized implosions [13] and affect the pinch dynamics [14]. Such effects can lead to significant magnetic flux losses, which may in turn lower the neutron yield. To study multi-dimensional, multi-physics effects in the SZP concept we must therefore turn to simulation codes that can furnish high-fidelity non-liner models.

In the context of the U.S. DOE ARPA-E BETHE program, MIFTI has established a collaboration with the theory/modeling Capability Team at the University of Rochester (PI Tzeferacos) that utilizes a suite of simulation codes – fluid, hybrid, and kinetic – to provide simulation support for ARPA-E Fusion Concept Teams. For this collaboration, the team is employing the FLASH code [15] to perform 1D simulations of the SZP concept and assess the feasibility and viability of the platform for fusion energy. This INFUSE project is a natural extension of that partnership, and has the following three research targets:

1. Develop and exercise FLASH's current drive unit in 3D Cartesian coordinates to execute high-fidelity 3D FLASH simulations of the SZP platform.
2. Model previously published SZP platform designs to assess the stability of the pinch (liner and target) to MHD instabilities.
3. Model previously published SZP platform designs and using all of FLASH's extended-MHD terms to assess how they affect implosion dynamics and plasma conditions at stagnation.

The results of research targets 2 and 3 are discussed in sections 2.1 and 2.2, whereas the results of target 1 are discussed in section 2.3.

1.3 The FLASH Code

FLASH [15] is a publicly available, parallel, multi-physics, adaptive mesh refinement (AMR), finite-volume Eulerian hydrodynamics and MHD code, we develop at the Flash Center (for more information on FLASH, visit: https://flash.rochester.edu). FLASH scales well to over 100,000 processors and uses a variety of parallelization techniques like domain decomposition, mesh replication, and threading, to optimally utilize hardware resources. The FLASH code has a worldwide user base of more than 4,500 scientists, and more than 1,300 papers have been published using the code to model problems in a wide range of disciplines, including plasma astrophysics, combustion, fluid dynamics, HED physics, and fusion energy.

Over the past decade and under the auspices of the U.S. DOE NNSA, the Flash Center has added in FLASH extensive HED physics and extended-MHD capabilities [16] that make it an ideal tool for the multi-physics modeling of the gas-puff Z-pinch experiments. These include multiple state-of-the art hydrodynamic and MHD shock-capturing solvers [17], three-temperature extensions [16] with anisotropic thermal conduction that utilizes high-fidelity magnetized heat transport coefficients [18], heat exchange, multi-group radiation diffusion, tabulated multi-material EOS and opacities, laser energy deposition, circuit models [19], and numerous synthetic diagnostics [20]. FLASH's newest algorithmic developments include a complete generalized Ohm's law that incorporates all extended MHD terms of the Braginskii formulation [21],

$$\begin{aligned}\mathbf{E} &= -\mathbf{u}\times\mathbf{B} + \frac{\mathbf{J}}{n_e e}\times\mathbf{B} - \frac{\nabla P_e}{n_e e} \\ &+ \frac{\eta_\parallel}{\epsilon_0\omega_{pe}^2\tau_{ei}}\mathbf{b}(\mathbf{b}\cdot\mathbf{J}) + \frac{\eta_\perp}{\epsilon_0\omega_{pe}^2\tau_{ei}}\mathbf{b}\times(\mathbf{J}\times\mathbf{b}) - \frac{\eta_\wedge}{\epsilon_0\omega_{pe}^2\tau_{ei}}(\mathbf{b}\times\mathbf{J}) \\ &- \beta_\parallel\mathbf{b}(\mathbf{b}\cdot\nabla T_e) - \beta_\perp\mathbf{b}\times(\nabla T_e)\times\mathbf{b}) - \beta_\wedge(\mathbf{b}\times\nabla T_e)\end{aligned}$$

where **E** is the electric field, **B** the magnetic field, **u** the plasma velocity, **J** the current density, n_e the electron number density, e the electron charge, P_e the electron pressure, **b** the unit vector in the direction of the magnetic field, ω_{pe} the electron plasma frequency, ε_0 the permittivity of vacuum, τ_{ei} the electron-ion collision time, T_e the electron temperature, and η and β are respectively the resistivity and the electrothermal coefficient in dimensionless form. The new extended MHD capabilities are integrated with new, state-of-the-art transport coefficients [22], developed with support from the U.S. DOE ARPA-E BETHE program.

The FLASH code and its capabilities have been validated through benchmarks and code-to-code comparisons [23-25], as well as through direct application to numerous plasma physics experiments [26-32], leading to innovative science and publications in high-impact journals. The Flash Center is also collaborating with Los Alamos National Laboratory (LANL) in the modeling of laser-driven experiments of cylinder implosions [33] at the Omega Laser Facility at the University of Rochester and the National Ignition Facility at Lawrence Livermore National Laboratory, in a successful integrated inertial confinement fusion (ICF) verification and validation (V&V) effort with xRAGE [34, 35].

For pulsed-power experiments, FLASH has been able to reproduce past analytical models [36], is being applied in the modeling of capillary discharge plasmas [37] and is being validated against gas-puff experiments at CESZAR at UC San Diego [38]. Extensive code-to-code verification efforts are also underway on gas-puff Z-pinch configurations, comparing FLASH simulations to MACH2 models on the SZP concept [39], discussed below, and to HYDRA models of two- and three-nozzle gas-puff Z-pinch configurations [40, 41].

2 Project Technical Activities

2.1 Code-to-code Comparisons on 1D SZP Simulations and Theory of Radiative Shocks in SZP

Primarily supported by the U.S. DOE ARPA-E BETHE program and in part by this INFUSE effort, the one-dimensional modeling of the SZP platform with FLASH has already furnished two articles that are currently under review [39, 42].

The paper first paper [39], which is in press in Physics of Plasmas and can be found in on ArXiv, is the first FLASH manuscript with full-physics simulations of pulsed-power experiments. The paper discusses the verification of FLASH and MACH2 codes using two analytical benchmarks that include Z-pinch-relevant physics, building confidence on the codes' ability to model such experiments. Then, FLASH is used to simulate two different SZP configurations: a xenon gas-puff liner (SZP1*) and a silver solid liner (SZP2). The SZP2 results are compared against previously published MACH2 results, and a new code-to-code comparison on SZP1* is presented (Figure 2). Using an ideal equation of state and analytical transport coefficients, FLASH yields a fuel convergence ratio (CR) of approximately 39 and a mass-averaged fuel ion temperature slightly below 1 keV for the SZP2 scheme, significantly lower than the full-physics MACH2 prediction. For the new SZP1* configuration, full-physics FLASH simulations furnish large and inherently unstable CRs (> 300) but achieve fuel ion temperatures of many keV. While MACH2 also predicts high temperatures, the fuel stagnates at a smaller CR. The integrated code-to-code comparison reveals how magnetic insulation, heat conduction, and radiation transport affect platform performance and the feasibility of the SZP concept.

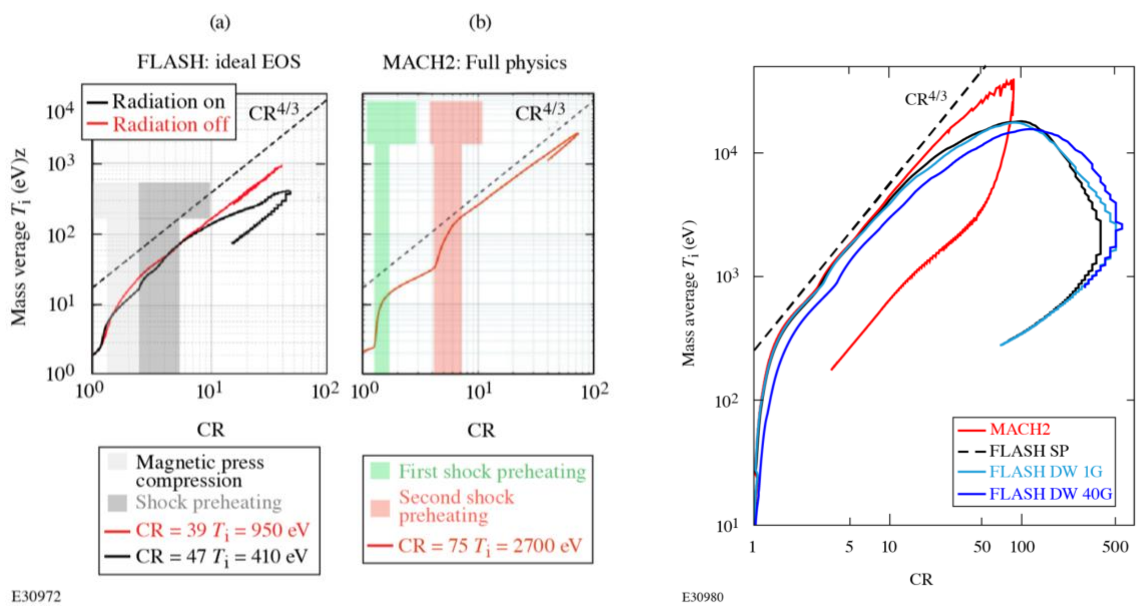

Figure 2. Left: Mass-averaged ion temperature vs. convergence ratio (CR) in the ideal-EOS FLASH SZP2 run (a) and full-physics MACH2 run (b) from Ruskov et al. (*Phys. Plasmas* 27, 042709, 2020), where SESAME tables were used. Right: Mass-averaged ion temperature vs. convergence ratio (CR) for all SZP1* simulations from FLASH and MACH2. The single-group FLASH run with Spitzer transport coefficients (SP) is directly comparable to the MACH2 run. The other FLASH runs used the newer transport coefficients (DW) and used either a single group (1G) or 40 groups (40G).

The second paper [42] looks at shock wave formation in radiative plasmas and its application to SZP implosions. More specifically, we investigate the temporal evolution of weak shocks in a radiative media. The structure of radiative shocks has traditionally been studied in a stationary framework and systematic classifications have proven to be complex as layers of optically thin and thick regions alternate to form precursor and relaxation regions, between which the hydrodynamic shock is embedded. In this work, we analyze the formation of weak shocks when two radiative plasmas with different pressures are put in contact. Applying a reductive perturbative method we recover a Burgers-type equation that governs the temporal evolution of the perturbed variables including the radiation field. The conditions upon which optically thin and thick solutions exist have been obtained and expressed as a function of the shock strength and Boltzmann number. Below a certain Boltzmann number threshold, weak shocks always become optically thick asymptotically in time, while thin solutions appear as transitory structures. The existence of an optically thin regime is related to the presence of an over-dense layer in the compressed material. Scaling laws for the characteristic time formation and length are provided for each regime. The theoretical analysis is supported by FLASH simulations. Based on the analysis, we investigate shock wave formation in gas-puff implosions with a high-atomic number liner. We identify the parameters for which the over-compression regime is relevant on the time and length scales characteristic of Z-pinch design-space (Figure 3).

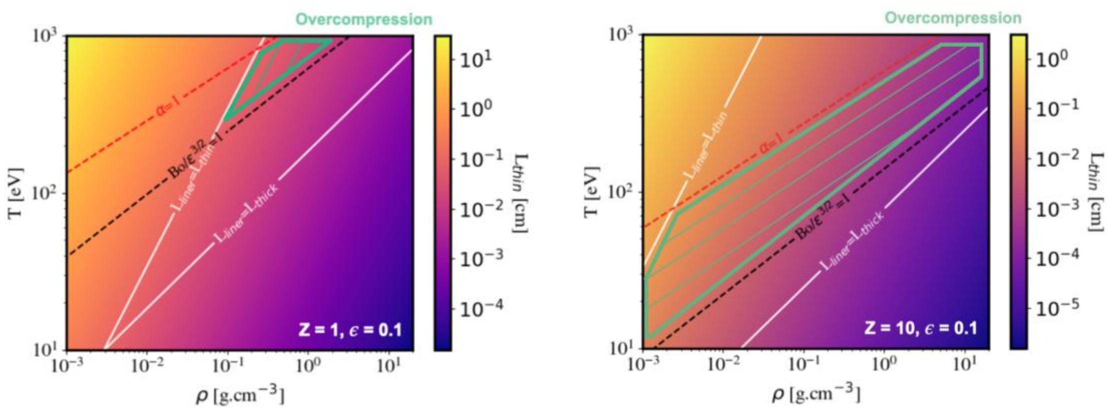

Figure 3. Isocontours of relevant parameters and lengths in the liner design space density- temperature. A liner thickness L_{liner} = 0.1 cm and a shock strength ε = 0.1 are considered. Left panel: Deuterium liner Z = 1. Right panel: Xenon liner with an ionization state Z = 10. The green shadowed region corresponds to the conditions in which such shock is radiation-dominated and optically thin, leading to over-compression. The red dotted line α = 1 corresponds to internal pressure equal to radiation pressure.

2.2 Two-dimensional SZP Simulations with FLASH to Study Stability – SZP Experiments

Simulating 2D gas puff Z-pinches is now possible with FLASH. Compared to the 1D simulations that were previously verified against the MACH2 code [39], 2D calculations are more challenging to perform. During liner-on-target implosions, the growth of the Rayleigh Taylor instability (RTI) can, in some cases, destroy the interface between the two materials. The adaptive mesh refinement technique implemented in FLASH allows us to perform high resolution simulations and thus capture well the dynamics of the instability. One of the main targets of study then becomes the RTI and its mitigation, without the use of axial magnetic fields.

The common wisdom is to use shorter and shorter radii for the liner, sometimes close to the millimeter scale, in an effort to limit the time in which the RTI could develop. However, recent experiments have been shown to be astonishingly stable when using particularly low density (~ μg cm^{-3}) and long liners (~ several cm). Similar experiments have been conducted by Conti et al. [43] on ZEBRA, and showed, without the use of stabilizing external magnetic fields that some RTI effects should be expected for liner radii of the order of 0.5 cm. Using FLASH, we wanted to assess what physical process stabilized the RTI and reproduced both configurations, in a first attempt to qualitatively reproduce the instability dynamics in these experiments.

To do that, 2D FLASH simulations were performed, using 3T MHD with a gray diffusion as a radiative transport model, coupled to state-of-the-art conductivity [18] and resistivity [22] coefficients. The setup uses multi-material equation of state and opacity tables, making it possible to simulate the Dt target plasma, the Ar liner plasma, and the pseudo-vacuum region through which the B-field driving the compression diffuses. The current profile comes directly from the published experimental results. However, for designing future experiments, we have implemented different circuit models in FLASH (see e.g., [19]). The axial mesh resolution is limited to ~ 0.1 mm to compare the simulations results at a resolution that matches the approximate dominant mode of RTI in the experiments. Finally, a 1-2% volumetric density perturbation is seeded inside the Ar liner to seed the RTI and mimic experimental variability.

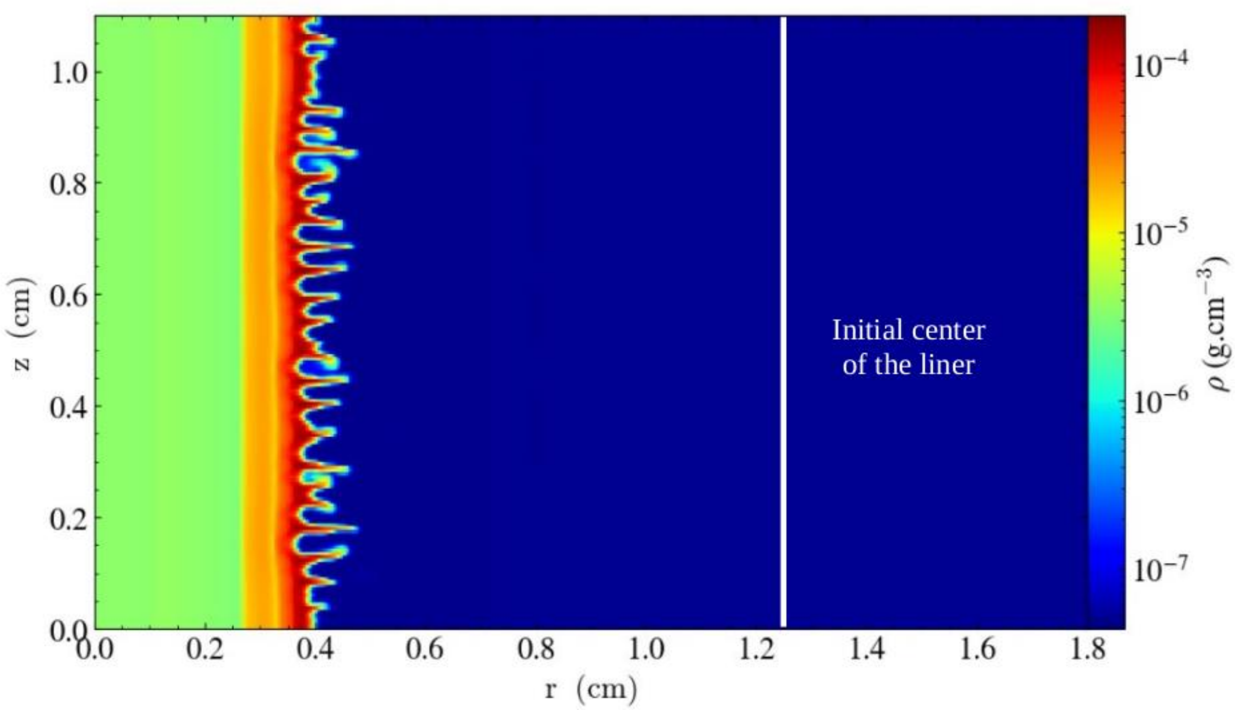

Figure 4. Density map of a 2D FLASH simulation of Conti et al. [43] experiments, taken at t = 95 ns, for a convergence ratio of 3.

The MHD solver used for the SZP simulations is HLLD, along with the third order PPM scheme, limited on the characteristic using the MC slope limiter. A coefficient of 0.1 is chosen for artificial viscosity, a common-used value for the PPM scheme. A CFL of 0.4 is imposed, ensuring numerical stability. All the diffusion processes, i.e., thermal conduction, radiation transport, and magnetic diffusion, are implicitly advanced, with, respectively, Larsen (coefficient 0.065), harmonic (coefficient 1.0) and no flux limiter. A harmonic average for resistivity on cell faces is used while an edge-based method is used for ohmic heating calculations. No other extended MHD terms are used for these simulations. Boundary conditions are defined as a circuit condition at maximum radius and axial symmetry at r = 0, whereas the top and bottom boundaries are reflective with Neumann conditions for conduction and magnetic diffusion.

The first results from simulating the Conti et al. experiments are shown in Figure 4. The RTI growth and implosion timing agree well with the experimental measurements. We see that the RTI appears during compression and starts to affect the liner-target interface as observed in the experiments. We also discovered a low density (~ 10 μg cm^{-3}) and moderate temperature (~ hundreds eV) thin zone at the interface, which appears to mitigate the growth of the instability, albeit not sufficiently to prevent late-time destruction of the interface. However, simulating recent staged Z pinches experiments on Double Eagle by MIFTI Inc., we discovered that the fielded wide-target/wide-liner configuration was remarkably stable, reaching particularly high temperatures in the target (~ 3 keV). Results are presented in Figure 5. Future work will therefore involve exploring the physics of the formation of such a mitigation region and the mechanisms that lead to stabilization of the pinch. Finally, a proposal to the ZNetUS program has been recently awarded to conduct ZEBRA experiments to validate FLASH and study the conditions in which liner and target extent can be leveraged to stabilize the RTI, like in the MIFTI Double Eagle experiments.

More work has also been performed to simulate staged Z pinches configurations studied previously by MIFTI with MACH2 [45] and explored recently in 1D with FLASH [39]. This 2D study investigated the numerical seeding of short-wavelength RTI modes when increasing mesh resolution, with a focus on how these modes can be damped (e.g., smoothing the density profiles between liner and vacuum, resolving of the dominant modes, assessing their scale, and artificial dissipation methods). A paper is currently being written on this subject [44] and some results are presented in Figure 6 for SZP1 and Figure 7 for SZP1*.

The first setup (SZP1) uses a small Xenon liner ($L = 0.2$ cm) with a Gaussian density profile ($\rho_{max} = 1.8 \times 10^{-1}$ g cm^{-3}) at 2 eV initial temperature, surrounding an uniformly filled Dt target ($R_{\text{targ}} = 0.3$ cm, $\rho = 3.4 \times 10^{-3}$ g cm^{-3}) at the same temperature. For the current drive, we used an RLC circuit model implemented in FLASH. The second setup (SZP1*) uses a larger Xenon liner ($L = 1.2$ cm) with a Gaussian density profile ($\rho_{max} = 3.5 \times 10^{-3}$ g cm^{-3}) at a 2eV initial temperature, surrounding a larger Gaussian Dt target ($R_{\text{targ}} = 0.5$ cm, $\rho = 3.5 \times 10^{-3}$ g cm^{-3}), at the same temperature. The latter was driven using the McBride et al. [19] circuit model, also available in FLASH. In both cases, the axial extent of the configuration is 1.5 cm whereas the two domains differ radially. A $1 - 2\%$ density perturbation is seeded in the liner to mimic plasma inhomogeneities.

Overall, SZP1 is more stable than SZP1*, which is a setup in which we reach higher implosion velocities and higher convergence ratios (Figure 8). However, the effect of high resolution on the stability of the simulations cannot be ignored. Work is ongoing on studying these two setups in detail to assess the effect of mesh resolution on the dominant mode of the RTI. The paper will detail how to produce such simulations.

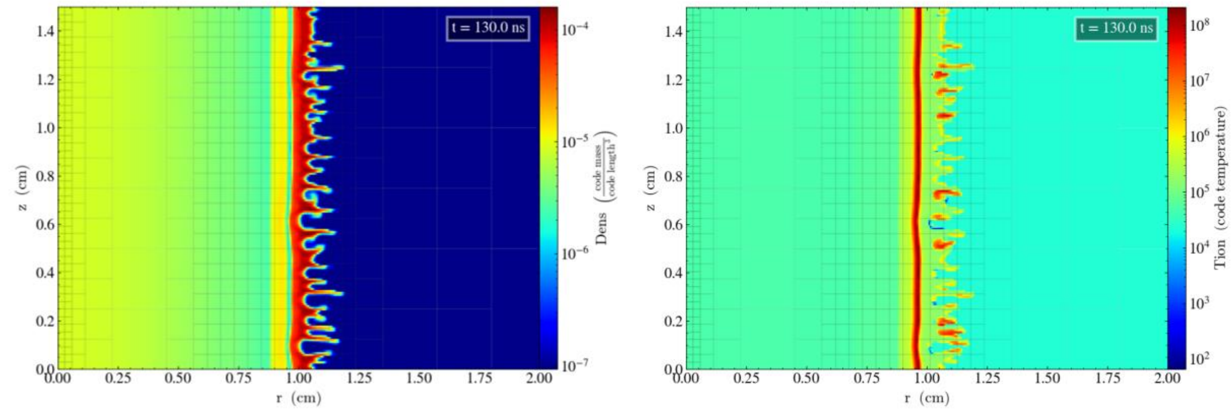

Figure 5. Density (left) and Temperature (right) map of a 2D FLASH simulation of Double Eagle experiment, taken at t = 130 ns, for a convergence ratio of 3. A low density and high temperature region is clearly seen. This will mitigate the instability, preventing it from entering the target, leading to an impressive stabilization of the pinch, as seen in the experiments.

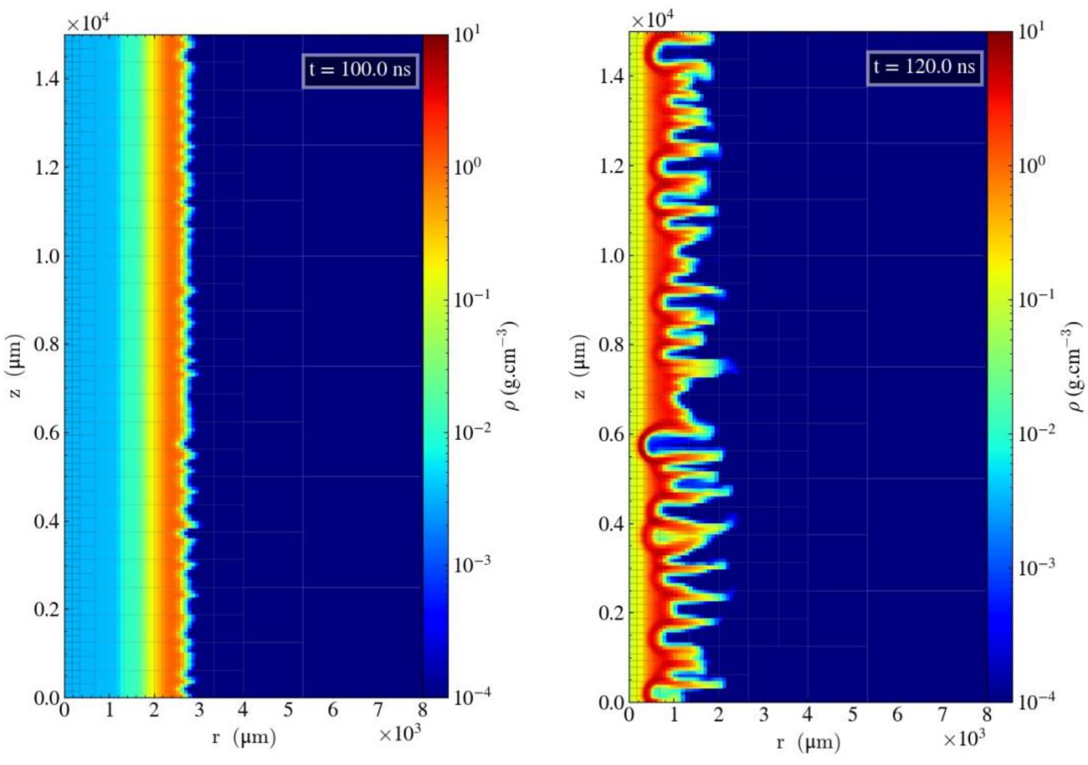

Figure 6. Density maps of a SZP1 simulation at t = 100 ns and t = 120 ns. RTI growth is particularly important in this setup which could degrade the implosion.

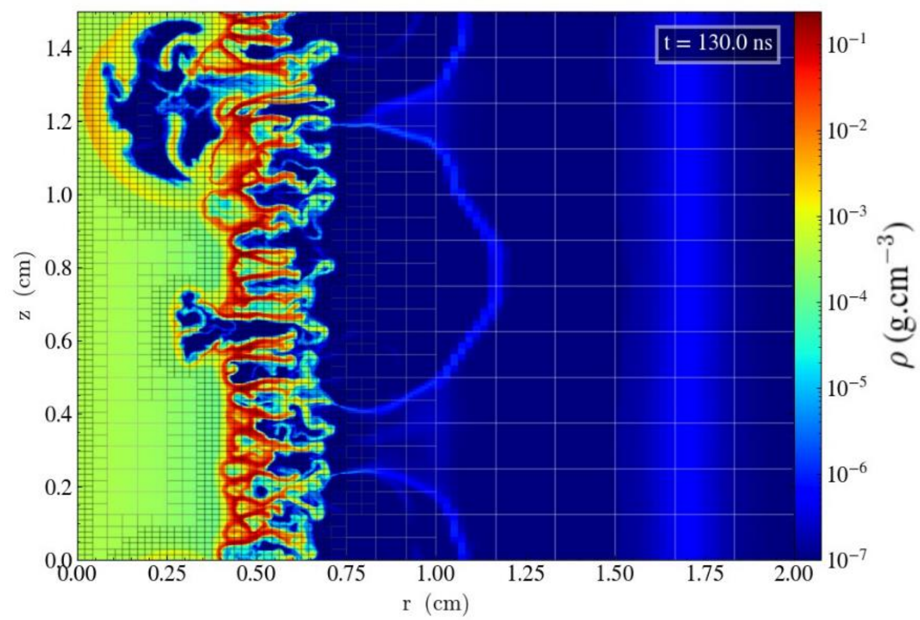

Figure 7. Density map of a high resolution (0.02 mm) SZP1* simulation at t = 130 ns. RTI growth is so important that, in the non-linear phase, the bubbles destroy the liner-target interface.

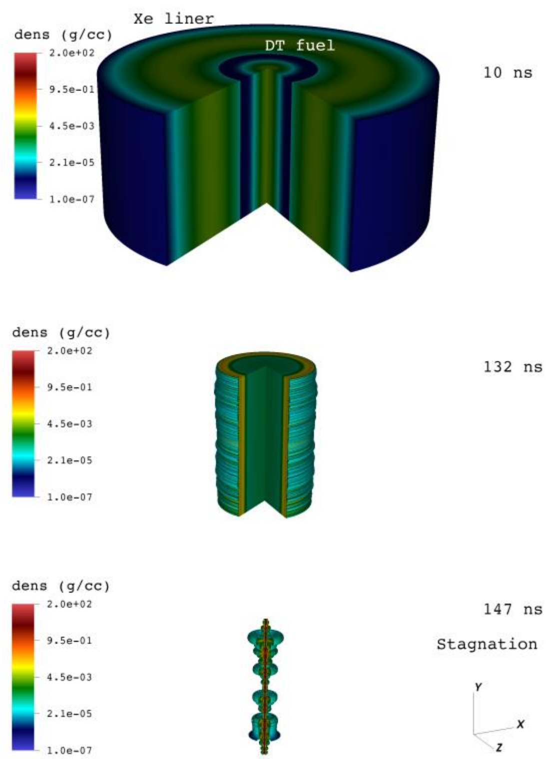

Figure 8. A sample 2D FLASH SZP1* simulation. Shown is the evolution of the density profile and the MRTI development, rendered in three dimensions by utilizing the cylindrical symmetry of the simulation.

2.3 Three-dimensional Z-pinch Simulations with FLASH

The core of simulating Z-pinch experiments is in modelling the current drive with a magnetic field boundary condition. Through Ampere's Law the enclosed current in the simulation domain is equivalent to an externally driven circuit model of the larger experimental apparatus. In this way the system can be modelled using MHD rather than needing to resolve the fast speed of light dynamics of the full Maxwell's equations, so long as the magnetic field in the simulated vacuum responds to changes in the current drive faster than any of the MHD timescales in the plasma.

This can be accomplished by specifying a magnetic field boundary condition from Ampere's Law at the edge of the simulation domain together with an artificially high magnetic resistivity in the simulated vacuum, causing the resistive MHD in the vacuum to diffuse the boundary field into the simulation domain at an arbitrary timescale set by the resistive diffusion. This is achieved by setting the vacuum resistivity to be orders of magnitude larger than the values in the plasma, which presents several difficulties in solving for stable and physical numerical solutions, particularly in multidimensional simulations.

The large separation in timescales between the vacuum magnetic resistivity and the dynamics of the implosion requires an implicit solver for the magnetic diffusion so that the simulation resolves only the timescales of interest rather than the arbitrarily fast vacuum field diffusion. Because of the possibility of adjacent cells having orders of magnitude different resistivity coefficients, the matrices that need to be inverted for the implicit solves have the potential to be poorly conditioned, which without careful construction can cause numerical instability and/or unphysical solutions.

In finite volume method (FVM) codes such as FLASH, the system of PDEs is cast as a conservation law such that solution variables may be explicitly conserved by considering the average flux through the center of bounding faces that join control volumes centered on the cells of the computational mesh.

$$\partial_t \int dV\, U(x,y) = -\oint d\boldsymbol{A} \cdot \boldsymbol{F} = \sum\nolimits_{faces} F_A \cdot A$$

For systems like the heat equation the fluxes are given by derivatives along the direction of the flux multiplied by a transport coefficient at the face, i.e., $F_A \cdot n_x = \kappa_{A_x} \partial_x T$. This requires only simple one-dimensional stencils and the coupling of cells sharing a face through their shared face coefficient, κ_{A_x}. However, for magnetic diffusion all the fluxes on a face are given by an additional derivative transverse to the face normal, for the flux of B_x in the *x*-direction

$$F_A \cdot n_x = \eta_{A_x}\left(\partial_x B_y - \partial_y B_x\right).$$

The transverse derivative requires an extended stencil including cells that share an edge with the one of interest in the transverse direction and couples through the normal face transport coefficient. Similarly in the reverse direction the coupling would be for the flux of B_x in the *y*-direction

$$F_A \cdot n_y = \eta_{A_y}\left(\partial_y B_x - \partial_x B_y\right).$$

In many applications where the resistivity is a smooth function of space the two face coupling coefficients would be of similar magnitude, i.e., $\eta_{A_x}/\eta_{A_y} \sim 1$, and the resulting matrices are easily solved with conventional iterative methods. However, for simulating current drive in a Z-pinch the coefficients necessarily will differ by many orders of magnitude, yielding very poorly conditioned matrices that iterative methods will struggle to solve, often leading to numerical instability and unacceptable error at the plasma-vacuum interface.

To overcome this, we developed a new discretization of the face-averaged finite-volume fluxes using a numerical quadrature over the cell-faces

$$\frac{1}{A_x}\int_A F\cdot dA_x \simeq \eta_{A_x}\,\partial_x B_y - \frac{1}{2}\left(\eta_{y+}\,\partial_y B_x|_{y+} + \eta_{y-}\,\partial_y B_x|_{y-}\right).$$

The new method makes use of transverse derivatives on a face evaluated at the centers of bounding edges on the face so that coupling between cells on the extended stencil is always through the transport coefficients at the shared edge ensuring that it is always symmetric to give well-conditioned matrices. To this end we have implemented a new HYPRE based diffusion solver in FLASH that uses edge-centered derivatives rather than face-centered ones as is common in conventional finite-volume discretization.

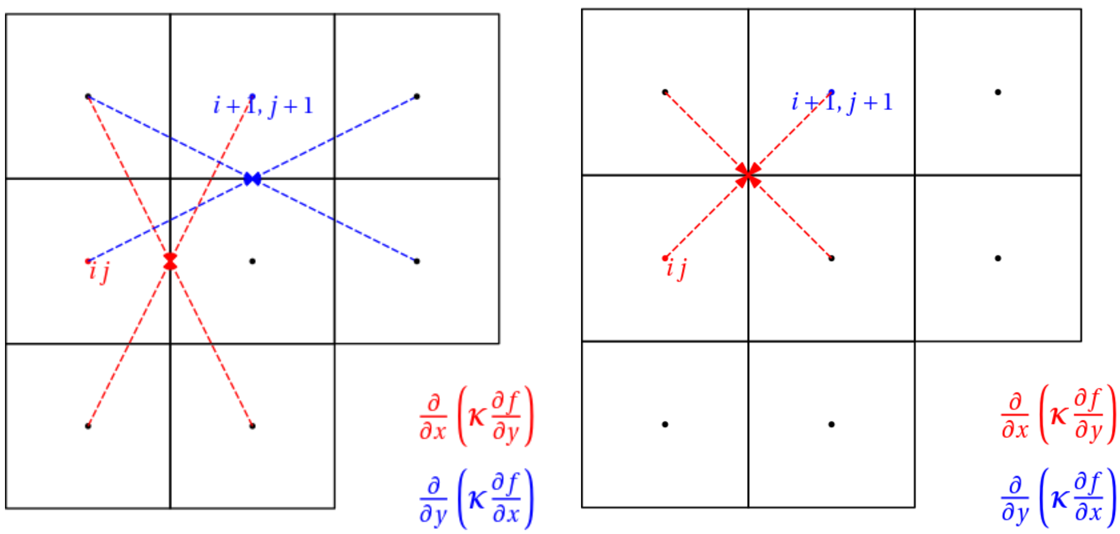

Figure 9. Stencil dependence for the different collocations of the derivatives along x (red) and y (blue) for the face-centered (left) and edge-centered (right) cases.

As a first test problem to assess FLASH's ability to simulate 3D Z-pinch configurations, we drive a 10 MA current through a solid Al wire in a 3D cartesian geometry (Figure 10). This is done by imposing an azimuthal magnetic field at the x & y boundaries of the domain, evaluated from Ampere's Law along with outflow boundary conditions in the z direction. The drive establishes a $1/r$ azimuthal field in the vacuum region with a constant current density field inside the wire. The magnetic field at the surface of the wire begins to compress the aluminum at the surface through the Lorentz force.

This INFUSE project has therefore enabled a new application domain for FLASH and furnished the academic pulsed-power HED communities with a publicly available simulation tool that can be used to design and interpret pulsed-power experiments.

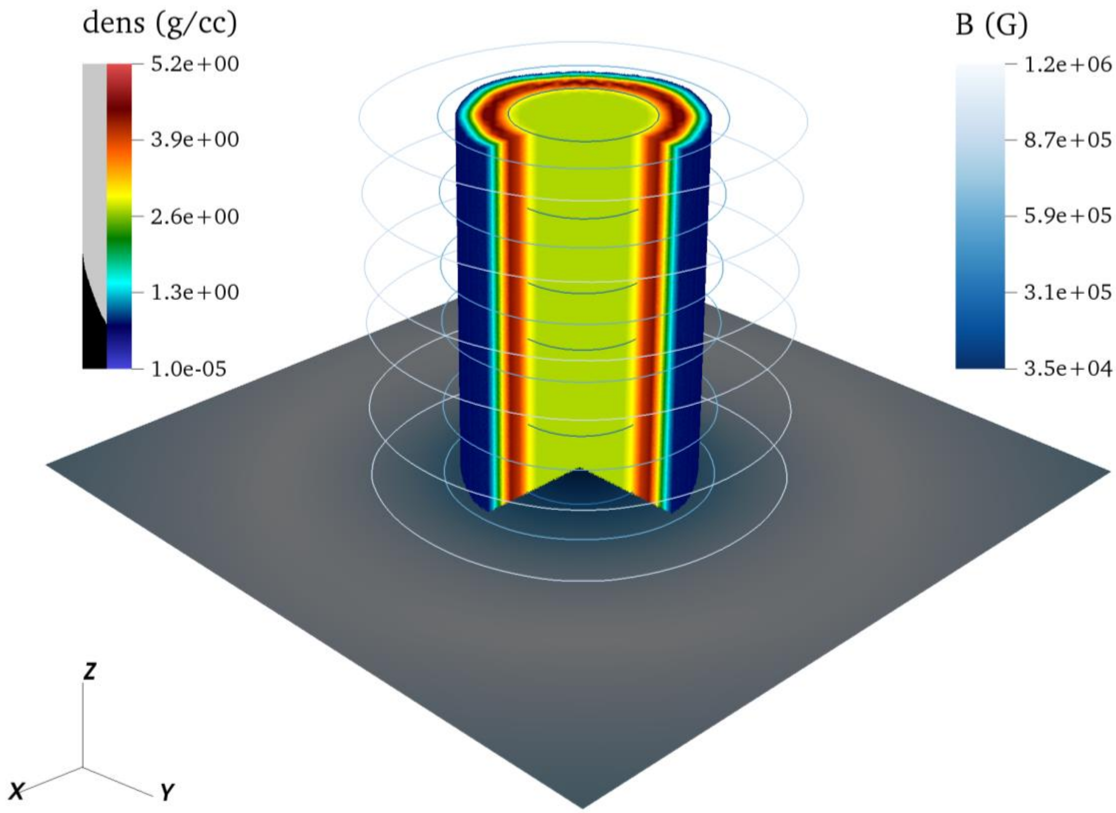

Figure 10. 3D Al wire implosion with FLASH. This is the first 3D Z-pinch simulation with the FLASH code. Shown are the 3D density profile resting on a 2D slice of the magnetic field and associated magnetic field contours.

4. Project Products

Work associated with this project has resulted in publications and presentations (invited and contributed talks, seminars, lectures, and posters), including the 65th APS-DPP Annual Meeting in Denver, CO. These are:

E. C. Hansen, F. Garcia-Rubio, M. B. P. Adams, M. Fatenejad, K. Moczulski, P. Ney, H. U. Rahman, A. C. Reyes, E. Ruskov, V. Tranchant, and P. Tzeferacos, "Feasibility and Performance of the Staged Z-Pinch: A One-dimensional Study with FLASH and MACH2", In Press, Phys. Plasmas.

F. Garcia-Rubio, V. Tranchant, E. C. Hansen, R. Tabassum, A. Reyes, H. U. Rahman, P. Ney, E. Ruskov, and P. Tzeferacos, "Shock Wave Formation in Radiative Plasmas and Application to Z-pinch Implosions", under review Phys. Rev. E.

F. García-Rubio, V. Tranchant, E. C. Hansen, A. Reyes, P. Ney, H. U. Rahman, E. Ruskov, and P. Tzeferacos, "Investigation of shock wave formation in radiative plasmas", Contributed talk at the 65th APS-DPP, Denver, CO, October 30-November 3, 2023.

V. Tranchant, E. C. Hansen, F. García-Rubio, K. Moczulski, A. Reyes, and P. Tzeferacos**,** "Studying Gas Puff Xe Liner Staged Z-Pinch stability with FLASH simulations", Contributed talk at the 65th APS-DPP, Denver, CO, October 30-November 3, 2023.

E. C. Hansen, F. García-Rubio, M. B. P. Adams, M. Fatenejad, K. Moczulski, A. Reyes, V. Tranchant, P. Ney, H. U. Rahman, E. Ruskov, and P. Tzeferacos, "*FLASH* Simulations of a Gas-Puff Xe Liner Staged Z-Pinch", Contributed poster at the 65th APS-DPP, Denver, CO, October 30-November 3, 2023.

C. L. Ellison, Keith LeChien, J. Carroll-Nellenback, F. Garcia-Rubio, E. Hansen, K. Moczulski, A. Reyes, and P. Tzeferacos, "Verification and Validation of FLASH for magnetized HED systems", Contributed talk at the 65th APS-DPP, Denver, CO, October 30-November 3, 2023.

P. Tzeferacos, A. Reyes, E. C. Hansen, F. García-Rubio, Y. Lu, D. Michta, R. Sarkis, A. Armstrong, K. Moczulski, P. Farmakis, A. Mohapatra, M. McMullan, T. Bachmann, A. Zou, J. P. Sauppe, A. Scopatz, and M. Fatenejad, "The FLASH code – an open simulation toolset for magnetized HED plasma physics and astrophysics", Invited poster at the SimNet Meet and Greet of LaserNetUS at the 65th APS-DPP, Denver, CO, October 30-November 3, 2023.

A. Reyes, E. Hansen, Jonathan Carrol-Nellenback, D. Michta, K. Moczulski, V. Tranchant, and P. Tzeferacos, "The FLASH code for computational HEDP – simulating pulsed power experiments," Invited talk at the ZNetUS Workshop, La Jolla, CA, January 8-10, 2024.

D. Michta, A. Reyes, E. C. Hansen, V. Tranchant, J. Carroll-Nellenback, B. Liu, R. Sarkis, A. Armstrong, K. Moczulski, P. Farmakis, A. Mohapatra, M. McMullan, A. Zou, J. Sauppe, A. Scopatz, M. Fatenejad, and P. Tzeferacos, "The FLASH code – an open simulation toolset for magnetized HED plasma physics and astrophysics," Contributed poster presentation at the NIF/JLF User Group Workshop, Livermore, CA, January 30-February 1, 2024.

V. Tranchant, E. C. Hansen, F. Garcia Rubio, H. U. Rahman, P. Ney, E. Ruskov and P. Tzeferacos, "Studying properties of radiative gas puff Z-pinches with the FLASH code," Contributed poster presentation at the Matter in Extreme Conditions for Magnetized Plasmas, Montgenèvre, France, February 3-10, 2024.

V. Tranchant, E. C. Hansen, F. Garcia Rubio, H. U. Rahman, P. Ney, E. Ruskova, A. Williams, O. Yang, F.N. Beg, and P. Tzeferacos, "Gas puff Z-pinches implosions with the FLASH code: Focus on radiation effects and Rayleigh-Taylor instability," Invited poster presentation at the 2024 NSF ECLIPSE meeting, Rochester, NY, April 7-9, 2024.

P. Tzeferacos, A. Reyes, E. C. Hansen, D. Michta, V. Tranchant, J. Carroll-Nellenback, B. Liu, R. Sarkis, V. Vaidya, A. Armstrong, K. Moczulski, P. Farmakis, A. Mohapatra, M. McMullan, T. Bachmann, Y. Zou, J. Sauppe, A. Scopatz, and M. Fatenejad, "The FLASH code – an open simulation toolset for magnetized HED plasma physics and astrophysics," Invited poster presentation at the 2024 NSF ECLIPSE meeting, Rochester, NY, April 7-9, 2024.

5. References

[1] Radionuclide production using a Z-pinch neutron source, US Patent 8,837,661 (2014).
[2] Staged Z-pinch for the production of high-flux neutrons and net energy, US Patent 9,839,111 (2017).
[3] E. Ruskov, P. Ney, and H. U. Rahman, Phys. Plasmas 27, 042709 (2020).
[4] H. U. Rahman et al., J. Plasma Physics 75, 749, (2009).
[5] F. J. Wessel et al., IEEE Trans. Plasma Sci. 43, 2463 (2015).
[6] F. J. Wessel et al., AIP Conf. Proc. 1721, 060002 (2016).
[7] M. H. Frese, Technical Report No. AMRC-R-874, Mission Research Corporation (1987).
[8] U. Shumlak and C. Hartman, Physical review letters 75, 3285 (1995).
[9] M. Haines, Plasma Physics and Controlled Fusion 53, 093001 (2011).
[10] J. M. Stone and T. Gardiner, The Astrophysical Journal 671, 1726 (2007).
[11] T. J. Awe et al., Phys. Rev. Lett. 111, 235005 (2013).
[12] M. Haines and M. Coppins, Physical review letters 66, 1462 (1991).
[13] J. R. Davies, R. Betti, P.-Y. Chang, and G. Fiksel, Phys.Plasmas 22, 112703 (2015).
[14] S. Chen et al., Plasma Phys. Control. Fusion 63, 115019 (2021).
[15] B. Fryxell et al., Astrophys. J. Suppl. Ser. 131, 273 (2000).
[16] P. Tzeferacos et al., High Energy Density Phys. 17, 24 (2015).
[17] D. Lee, J. Comput. Phys. 243, 269 (2013).
[18] J.-Y. Ji and E. D. Held, Phys. Plasmas 20, 042114 (2013).
[19] R. D. McBride et al., Phys. Rev. Special Topics-Accelerators and Beams 13, 120401 (2010).
[20] P. Tzeferacos et al., Phys. Plasmas 24, 041404 (2017).
[21] S. I. Braginskii, Rev. Plasma Phys. 1, 205 (1965).
[22] J. R. Davies, H. Wen, J.-Y. Ji, and E. D. Held, Phys. Plasmas 28, 012305 (2021).
[23] M. Fatenejad et al., High Energy Density Phys. 9, 63 (2013).
[24] C. Orban, M. Fatenejad, S. Chawla, S. C. Wilks, and D. Q. Lamb, arXiv:1306.1584 (2013).
[25] C. Orban, M. Fatenejad, and D. Q. Lamb, Phys. Plasmas 29, 053901 (2022).
[26] J. Meinecke et al., Nat. Phys. 10, 520 (2014).
[27] J. Meinecke et al., Proc. Natl. Acad. Sci. U. S. A. 112, 8211 (2015).
[28] C. K. Li et al., Nat. Commun. 7, 13081 (2016).
[29] P. Tzeferacos et al., Nat. Commun. 9, 591 (2018).
[30] L. E. Chen et al., Astrophys. J. 892, 114 (2020).
[31] A. F. A. Bott et al., Proc. Natl. Acad. Sci. U. S. A. 118, e2015729118 (2021).
[32] J. Meinecke et al., Sci. Advances 8, eabj6799 (2022).
[33] J. P. Sauppe et al., Phys. Rev. Lett. 124, 185003 (2020).
[34] M. Gittings et al., Comput. Sci. & Discovery 1, 015005 (2008).
[35] J. P. Sauppe et al., Physics of Plasmas 30, 062707 (2023).
[36] S. A. Slutz et al., Phys. Plasmas 8, 1673 (2001).
[37] N. M. Cook et al., J. Phys.: Conf. Ser. 1596, 012063 (2020).
[38] F. Conti et al., Phys. Rev. Accelerators and Beams 23, 090401 (2020).
[39] E. Hansen et al., In Press arXiv:2311.07755 (2023).
[40] J. Narkis, F. Conti, A. L. Velikovich, and F. N. Beg, Phys. Rev. E 104, L023201 (2021).
[41] D. Michta et al., In Preparation.
[42] F. Garcia-Rubio, et al. Under Review (2023).
[43] F. Conti et al., Phys. Plasmas 27, 012702 (2020).

[44] V. Tranchant et al., In Preparation.
[45] H. Rahman et al. Journal of plasma physics 75, 749 (2009).