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COUPLING OF CODES FOR MODELING HIGH-ENERGY-DENSITY CONDITIONS IN FOURTH GENERATION LIGHT SOURCES *

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Abstract

We present a code coupling methodology of three simulation codes for particle dynamics (`elegant`), particle-matter interaction (FLUKA), and hydrodynamics (FLASH) to model the effects of high-intensity electron beams in fourth-generation storage rings for the purpose of machine protection. Nonlinearly combined, the coupled codes determine if high-energy-density conditions are present in beam-intercepting components. The code `elegant` is used to simulate the dynamics of a whole-beam abort within the APS (Advanced Photon Source) ring. The impacting electron beam particles begin interacting with a horizontal collimator, at which point in our simulations `elegant` is interrupted and the beam impact process is modeled using FLUKA and FLASH. FLUKA simulates the interaction of the beam with the collimator, passes the energy density deposition to FLASH, and returns the transmitted surviving particle distribution to `elegant`. Taking the FLUKA energy deposition as input, FLASH calculates the density evolution of the collimator material by considering the *emulated* proxy phase changes from solid to liquid and liquid to plasma. In the APS storage ring, the surviving beam is propagated again through the APS lattice, and the process is repeated until the beam is fully lost. The input FLUKA geometry is updated at each step to reflect the changing material properties of the beam and the collimator.

INTRODUCTION

The high-energy-density (HED) conditions (energy densities > 100 J/mm^3) present in fourth-generation light sources introduce a potential for machine damage and irradiation due to beam impacts with machine components. At design brightness, beam loss events can risk significant damage to the collimators intended to safely capture lost particles. Several studies have investigated these beam impacts as well as potential mitigation schemes [1–3].

An essential set of physics for modeling a beam impact event includes the simulation of (i) particle dynamics, (ii) particle-material interactions, and (iii) thermodynamic/hydrodynamic response of materials. Particle tracking codes, such as `elegant` [4], are widely used to simulate particle dynamics in storage rings and beamlines. There are also many particle-matter interaction codes, such as MARS [5] and FLUKA [6], that model the nuclear interaction and particle showers in matter. Although the aforementioned simulations of particle dynamics and particle-matter interactions are commonly used in accelerator and collider design, the final step in (iii) of modeling the hydrodynamics of irradiated accelerator beamline components is less commonly adopted. We seek to capture this (magneto)hydrodynamical response in a self-consistent way using the unsplit staggered mesh (USM) magngetohydrydynamics (MHD) solver [7, 8] of the publicly available software FLASH [9]. For this study we use the FLASH code version 4.7 that includes the suite of high-energy-density capabilities described in [10].

Yet, when combining these codes into a single code framework, a computational challenge quickly arises: these codes do not readily interface with each other because these software tools were originally developed to address each domain-specific physics. In order to have a useful, general-purpose predictive tool to simulate HED conditions in storage rings, they must be made to work together to best follow the nonlinear sequences of physics in the storage ring experiments. This paper outlines the initial steps toward developing a fully coupled code framework that allows each component to feed back on one another as well as demonstrating its capabilities on an experimentally studied case.

CODE COUPLING

In order to account for the changing environment of beam impact events, we developed a method of coupling three physics codes; `elegant`, FLUKA, and FLASH, to dynamically capture the beam and material evolution.

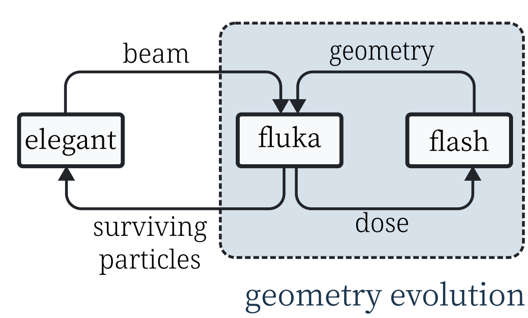

Figure 1: Diagram of the simulation coupling. Particle dynamics through the APS lattice are handled all at once by `elegant`. The geometry feedback between FLUKA and FLASH can occur multiple times within a single pass.

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In our study, we are primarily concerned with two properties of the system: (i) the change in geometry of the impacted collimator surface (i.e., surface erosion) and (ii) the change in particle transmission and energy deposition due to the eroded collimator material. The basic simulation structure is shown in Fig. 1. As energy is deposited into the material, it may be heated to the point of melting or vaporization. The changing material properties will affect the dose absorbed by the material at later time steps. As the collimator material is vaporized, particle transmission increases while deposition correspondingly decreases due to the eroding cross-section.

Geometry Evolution (FLUKA+FLASH)

In previous simulations of collimator impact events at APS, the material was treated as static when computing the energy deposition. Experimental studies of collimator impact exhibit both collimator surface erosion and longer beam lifetime than would be predicted from a static dose approximation, motivating the need for dynamics modeling capabilities.

We leverage the FLUKA code for modeling the beam-collimator interaction and the FLASH code for evolving the collimator material in response to the deposited energy and the resulting thermal property changes (e.g., melting and vaporization). Both codes run on a rectangular voxel (or mesh) structure. Our 3D simulations are configured on a 3D computational domain that spans the region $[-2.40, -1.90] \times [2.73, 3.03] \times [90, 110]$ (mm). The domain is common for both FLUKA and FLASH to enable the simulation setup to transfer density and dose information between the two codes on the same consistent grid geometry. The grid resolutions are listed in Table. 1.

Table 1: Properties of the simulation grid shared between FLASH and FLUKA. Simulations are conducted on a uniform mesh with grid resolutions of $N_{\text{grid}} = 128$ in both the x and y directions and $N_{\text{grid}} = 20$ in the z direction. Δ_{grid} is the corresponding grid length scale in each direction.

Coordinate	Min (mm)	Max (mm)	N_{grid}	Δ_{grid} (μm)
x	-2.40	-1.90	128	3.906
y	2.73	3.03	128	2.344
z	90.0	110.0	20	1000.0

The simulation geometry comprises 20 longitudinal z-slices with 128 horizontal rectangular box regions in each x-y cross section. Each horizontal x-y cross section region initializes the collimator boundary. For example, Fig. 2(a) shows the collimator phase boundaries at the center apex location (z = 100 mm), partially through the fourth turn.

The geometry can be updated in FLUKA multiple times per pass, even down to the individual bunch, allowing FLUKA to recompute the dose (Fig. 2(b)) and particle loss as the collimator is damaged by the FLASH calculation. Such updated dose map distributions are given to FLASH as part of the coupled geometry feedback between FLUKA and FLASH (see Fig. 1).

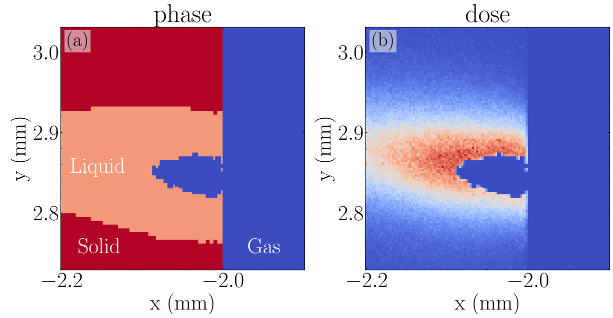

Figure 2: x-y cross section at the collimator center (z = 100 mm) after the 16th bunch out of 48 of the fourth pass (or turn) at t = 1.23×10^{-5} seconds, showing (a) the FLASH/FLUKA collimator geometry regions, and (b) the dose deposited by the electron beam showing that zero energy (colored in blue) is deposited in regions where there is no material due to evaporation. In (a), the color map displays the solid collimator material in red, the melted liquid material in coral, and the gas in blue. The blue region represents a "trenched" region where the initially solid material is vaporized to gas. In both (a) and (b), any liquid and gas regions in $x \leq -2.0$ show the changes of the collimator material from solid to liquid (melting) and liquid to gas (vaporization).

Particle Beam Dynamics (`elegant`+FLUKA)

The beam dynamics through the rest of the APS ring are tracked using `elegant`. A SCRIPT element is inserted in the APS lattice at the beginning of the collimator region, which exports the phase space coordinates of the whole beam. The beam distribution is fed into FLUKA, and any particles that reach the end of the simulation domain above an energy threshold (E_{min} = 0.98 E_0 = 5.88 GeV) are returned to `elegant`. As the collimator is eroded, some particles may pass through regions that were previously solid material. This effect can extend the duration of the beam loss as it will take more revolutions for all of the particles to strike the collimator.

SIMULATION RESULTS

Total Beam Loss

Using the fully coupled model described above, we simulated the impact of a 200 mA, 6 GeV electron beam on a copper collimator. The beam is initially at equilibrium in the APS ring; the rf cavities are then muted to initiate the beam abort. The first call to FLUKA is made when the beam begins to interact with the collimator (∼ 20 turns after the rf is muted). The FLUKA-FLASH loop runs six times within a single turn (or pass) to update the geometry as the collimator changes phase from solid to liquid and then liquid to gas. The physical properties of the collimator at the end of several turns are shown in Fig. 3. These results show the effect of the collimator surface being eroded by the incident beam. The electron temperature of the collimator gradually rises until the collimator surface begins to melt during the second turn. When the temperature at any grid cell (or voxel) exceeds 1.5 times the copper evaporation temperature, i.e., T_e = 1.5 T_{vap}, FLASH releases the cell from its solid state

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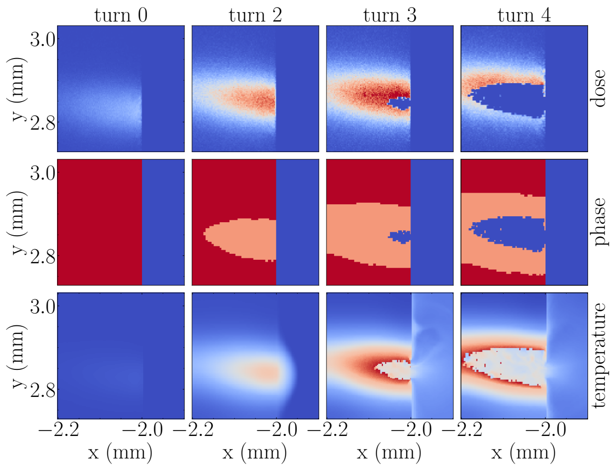

Figure 3: Evolution of dose (top), phase change (middle), and electron temperature (bottom) of the collimator during a beam loss event over 8 turns with 6 intra-turn feedback steps. Turn 1 results are omitted here as there is no phase change observed.

to an evaporated copper gas state, and the cell is evolved hydrodynamically in FLASH. The resulting vaporized region can be seen as "trenched" in the dose map, and the incident beam will no longer interact with those vaporized regions.

As the geometry evolves, FLUKA continuously updates the dose map as well as recomputes particle transmission. Figure 4 shows the effect of updating the geometry in this way on the rate of beam loss per turn. Initially the beam loss matches the static case until the material starts to vaporize around the third turn (or pass). The beam loss predictions start to deviate significantly from each other for the third turn and beyond. The evolving geometry calculation produces a skewed distribution that is more consistent with what was observed during experiments.

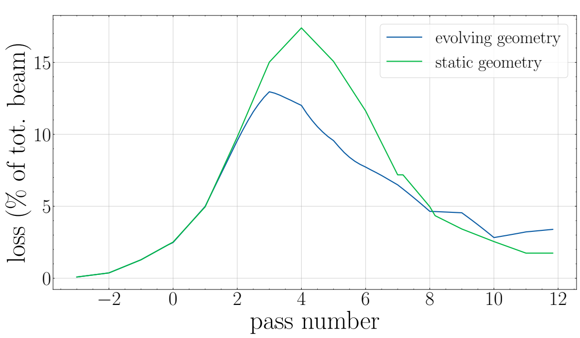

Figure 4: Comparison of the beam loss at each turn (or pass) for the cases of static geometry (green) and evolving geometry (blue) using the FLASH-FLUKA feedback loop.

Fan-Out Kicker Mitigation

One method proposed to mitigate the damage caused by a beam loss event is the use of a transverse deflecting fan-out kicker [11]. This scheme uses vertical deflection to move the beam across the collimator while nonlinearities in the fields defocus and inflate the beam, thereby spreading out the energy concentration deposited in the collimator. An example of the particle distribution on the collimator surface is shown in Fig. 5. The fan-out kicker scheme further demonstrates the need for finer temporal resolution when updating the collimator geometry. Each bunch in the beam will strike the collimator at a different vertical position due to the magnitude of the kick it receives. This stratification can be seen in Fig. 5(a), where the transverse distribution of the beam at the collimator position is plotted in blue streaks. The FOK pulse is a half sine wave over one turn yielding a peak deflection of 200 μrad.

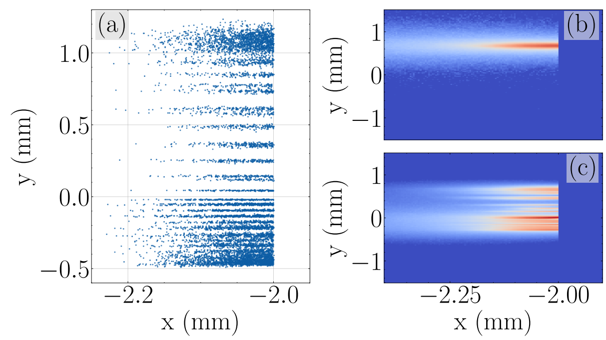

Figure 5: (a) Transverse distribution of all particles striking the collimator in a single pass (or turn), (b) dose map of a single bunch, and (c) dose map of the full pass (or turn), all with the FOK active.

CONCLUSION

This work presents a method of coupling three codes, the beam-dynamics code `elegant`, the particle-matter interaction code FLUKA, and the hydrodynamics code FLASH into a single unified workflow. This scheme will be critical for designing and operating future fourth-generation light sources. Data collected during three experimental studies of collimator beam strikes will serve as important benchmarks when validating these simulations.

While these initial results show encouraging agreement with experimental data, there are still several features which, if implemented in FLASH, would greatly improve the simulation accuracy. These include, (i) improving the handling of the liquid phase by evolving it hydrodynamically, (ii) phase boundary (solid-liquid-gas) tracking using a sharp interface-resolving method, (iii) a model of latent heat for phase changes, (iv) induced magnetic fields around the collimator surface, and (v) MHD effects due to induced fields. In future work we will investigate these potential improvements by integrating an immersed boundary method to advance our simulation predictability. Moreover, the electromagnetic effects will be integrated into the immersed boundary method to better handle the plasma-solid boundary conditions, which is crucial to maintain physical consistency in FLASH's USM-MHD solver [7, 8].

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