Coupled Simulations of Collimator Irradiation in Fourth Generation Light Sources

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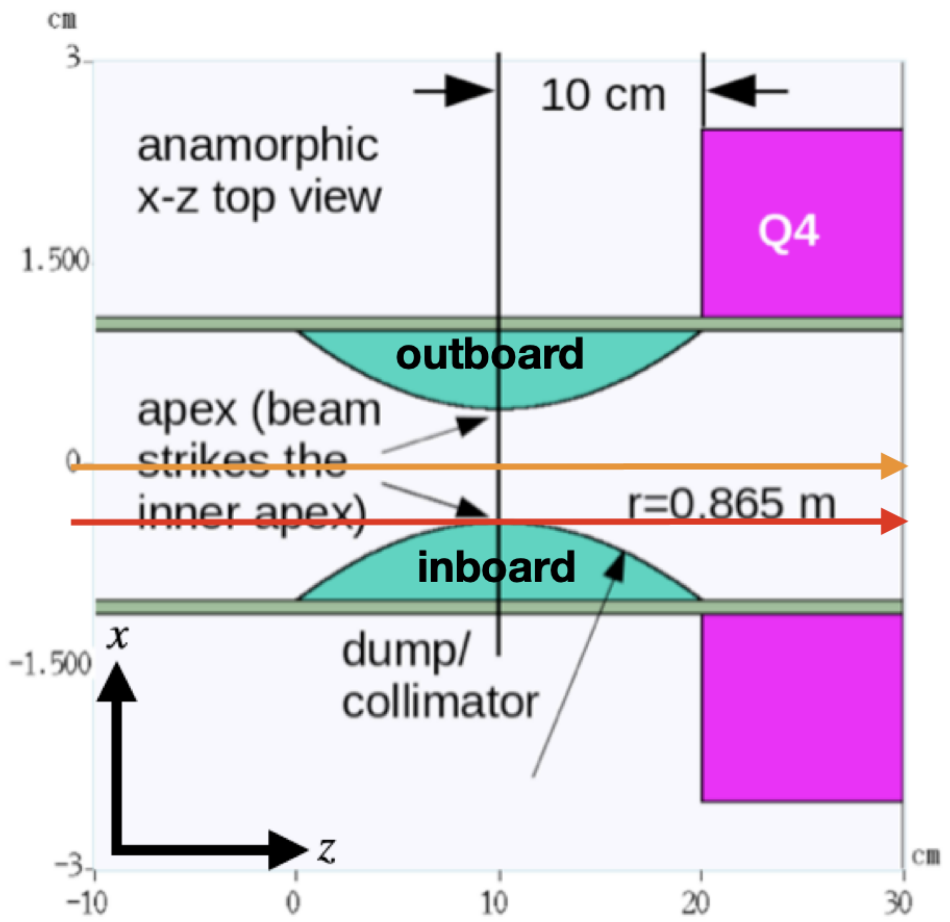
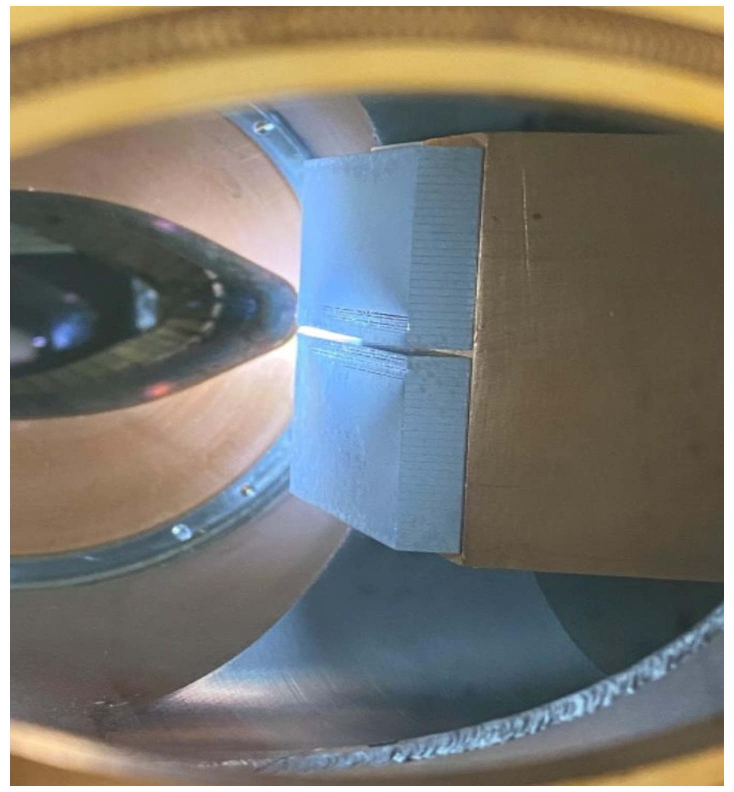
Fourth Generation Light Sources Compromise Machine Protection

- Beam intensity in 4th generation light sources threatens machine protection in the event of a whole beam abort

- APS-U promises a 70-fold increase in beam brightness
  - Significant reduction in horizontal beam size via multi-bend achromat lattice upgrade along with injection improvements
  - Stored current will also increase by a factor of 2 for some modes
  - Swap-out injection presents new risks during operation

- APS-U features beam abort collimator system to intercept particles in the event of a sudden loss event
  - RF system is tripped to steer beam towards inboard collimator protrusion
  - Vertically-translatable collimators enable variable capture of particles ahead of high priority sectors
  - Collimators are positioned to localize radiation in regions of maximum shielding



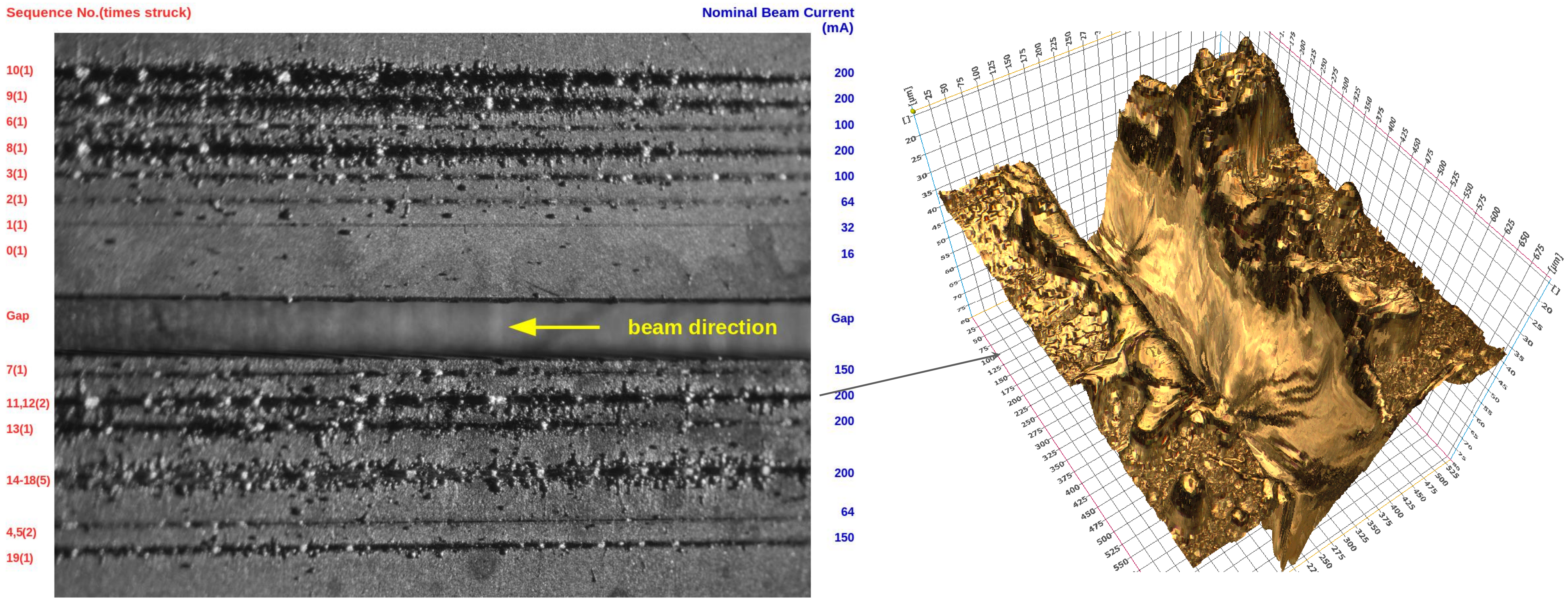


Collimator inside of vacuum chamber

Experiments Indicate Significant damage to collimators for high brightness beams

- Significant damage to collimators is expected under nominal beam incidence
  - Variations in fill pattern and operating current will modify observed damage
  - Variations in collimator material can be effective in modifying damage patterns
  - Images indicate melting, fluid flow, and condensation of material following beam strike

Increasing beam current, turn #



Evaluation and prediction of collimator performance requires multi-physics modeling

- Multi-faceted dynamics of beam strikes requires multi-physics models for complete understanding
  - Beam dynamics within the ring
    - Need electron dynamics including accurate transverse profile under varying fill patterns, RF response, and scattering
  - Beam-dose deposition
    - Particle-matter interaction codes can capture relevant energy loss and subsequent deposition in collimator
  - Collimator material response
    - Material-specific ionization, heating, dissipation, phase change, and advection
  - Other physics of interest
    - Magnetic field effects, including magnetohydrodynamics and wakefields
    - Radiation propagation downstream of the interaction can affect other compensation tools
- Complementary efforts to understand requirements for LHC tertiary collimators
  - Tertiary collimators protect critical IPs
  - Three-steep simulation approach
    - Particle tracking of proton beams with `SIXTRACK`
    - Energy deposition calculations with `FLUKA`
    - Hydrodynamic simulations of thermomechanical response via `AUTODYN`

E. Quaranta *et al.*, Phys. Rev. Accel. Beams **20**, 091002 (2017) DOI: 10.1103/PhysRevAccelBeams.20.091002

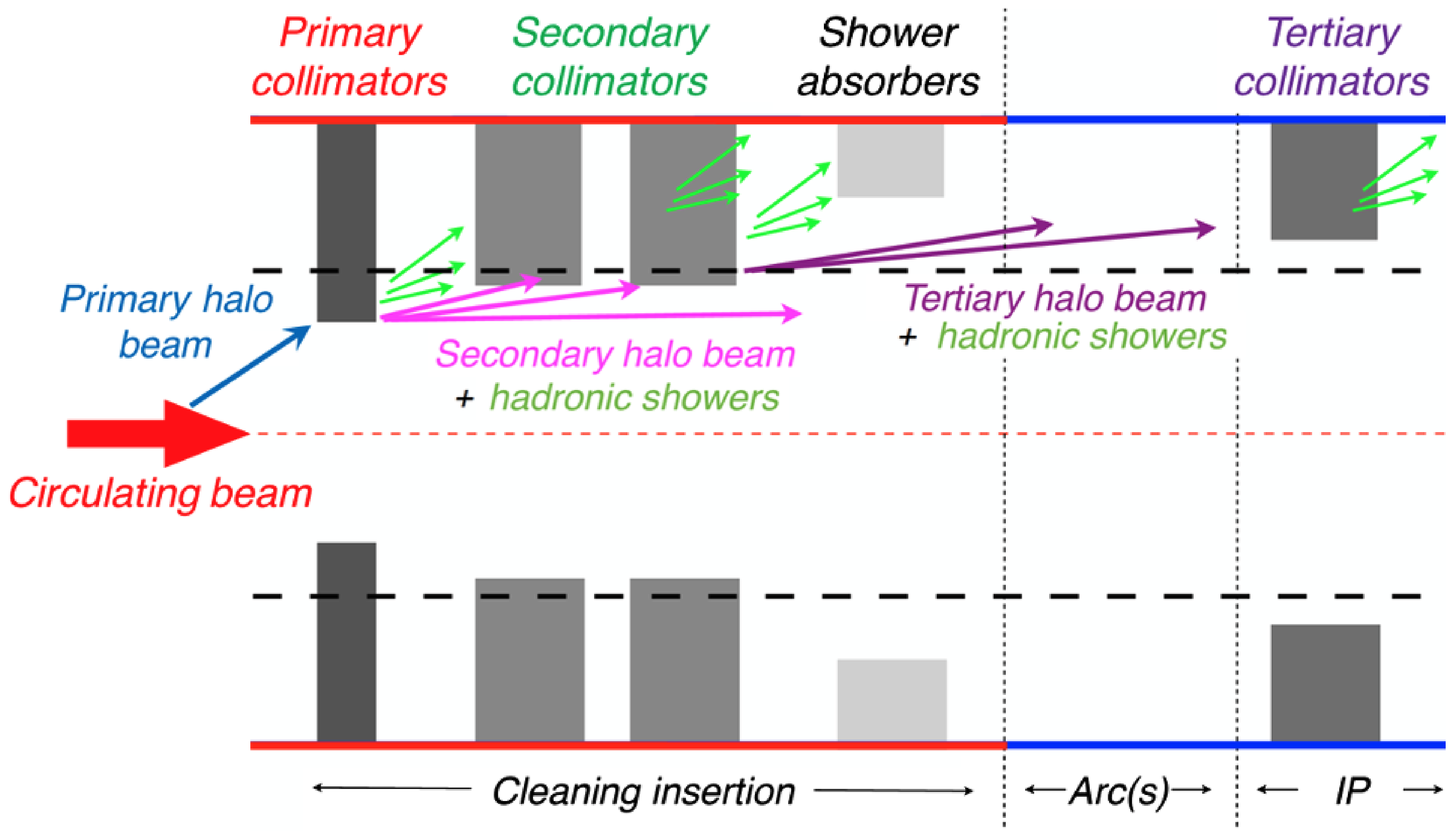
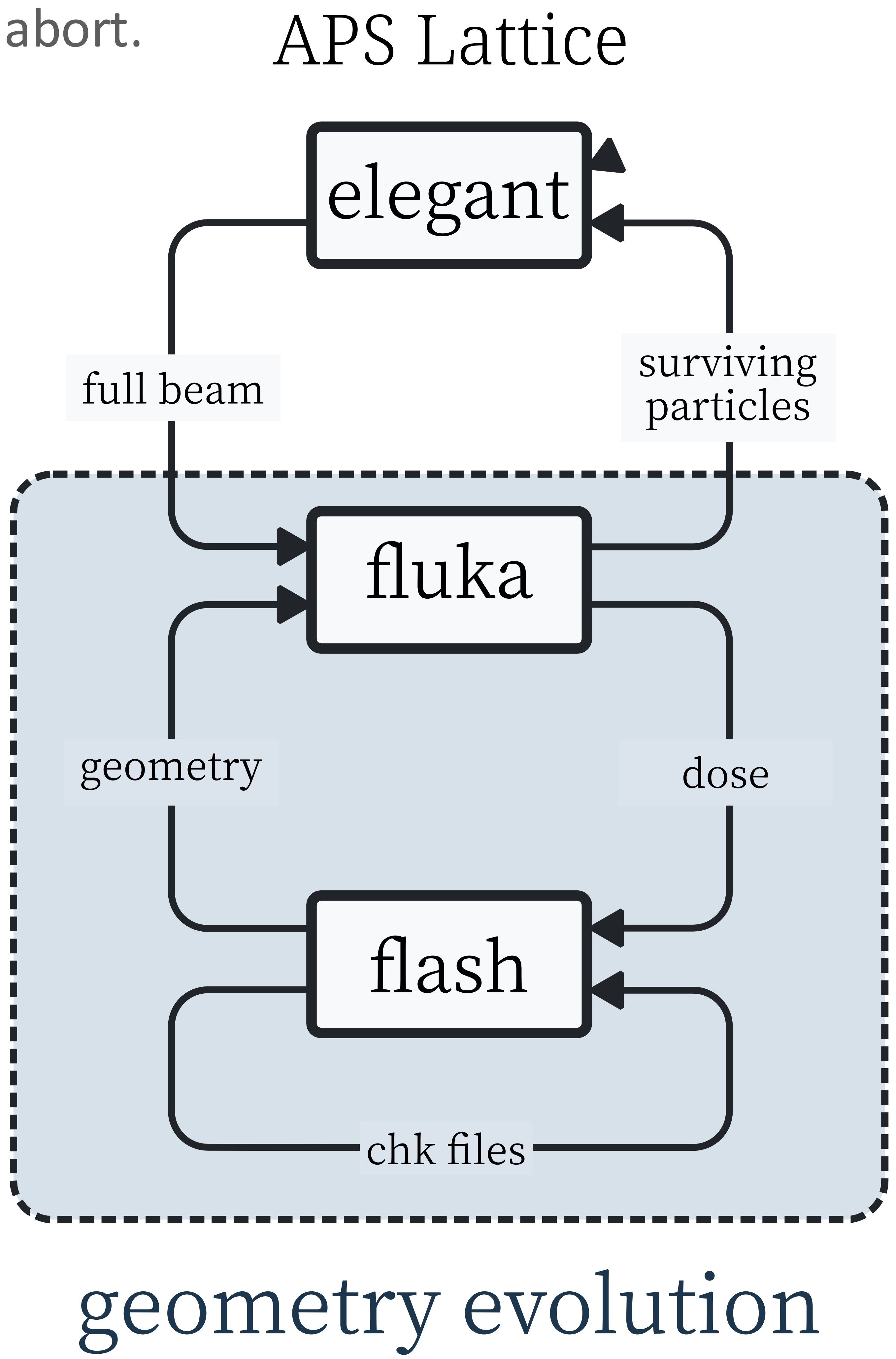


FIG. 3. Scheme of the collimator hierarchy in the LHC.

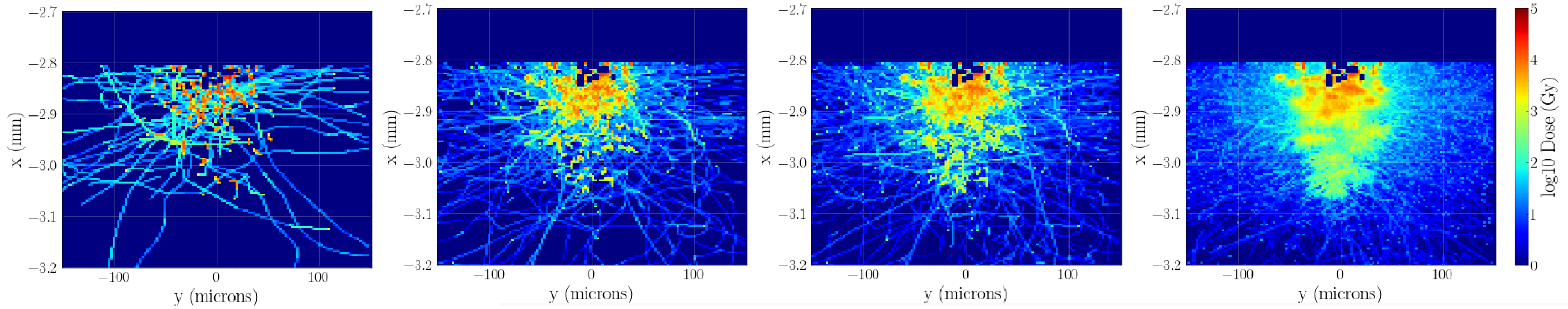
A simulation cycle for self-consistent collimator irradiation

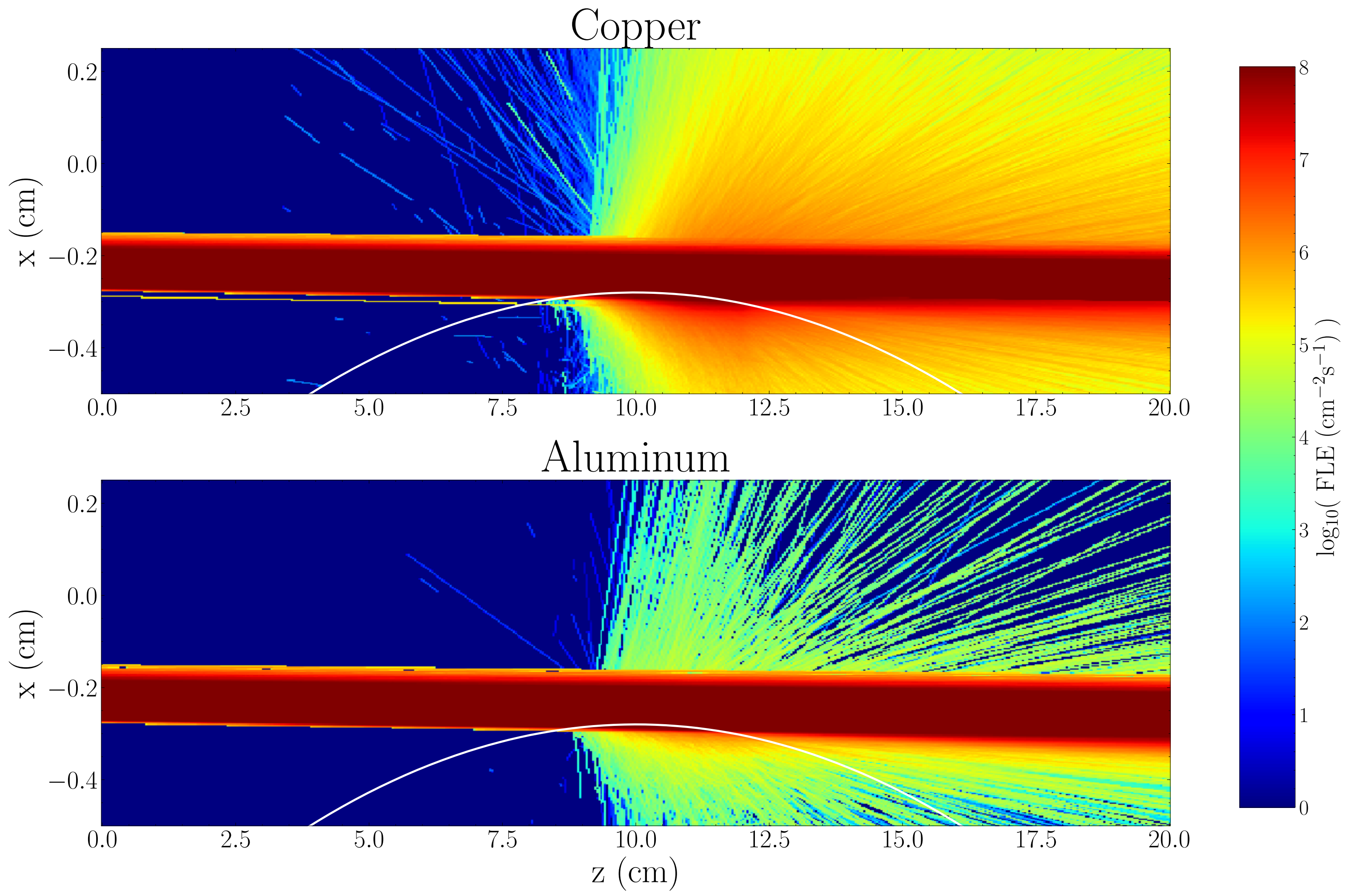
- Three-code coupling permits self-consistent spatiotemporal evolution of collimators
  1. `elegant` provides particle dynamics
     1. Tracks beam through APS lattice, including RF dynamics resulting from simulated abort.
     2. Outputs beam coordinates at the collimator surface entrance
  2. `FLUKA` provides particle-matter interaction
     1. Monte-Carlo estimation of particle losses
     2. Multiple Coloumb scattering, bremmstrahlung, pair production
     3. Produces a 3D map of the energy deposition (resolution can be varied)
     4. Returns coordinates of surviving source particles for `elegant`
  3. FLASH provides (magneto)hydrodynamics response of collimator
     1. Translates energy deposition into corresponding state variables.
     2. Computes thermal (and magnetic) transport through materials
     3. Enables identification of phase changes via user-specified models
     4. Subsequently, advects materials in fluid state and updates transport
- FLUKA–FLASH subloop enables repeated estimation of deposition and corresponding evolution within a single pass
  - Inter-bunch dynamics for varying fill patterns can be captured

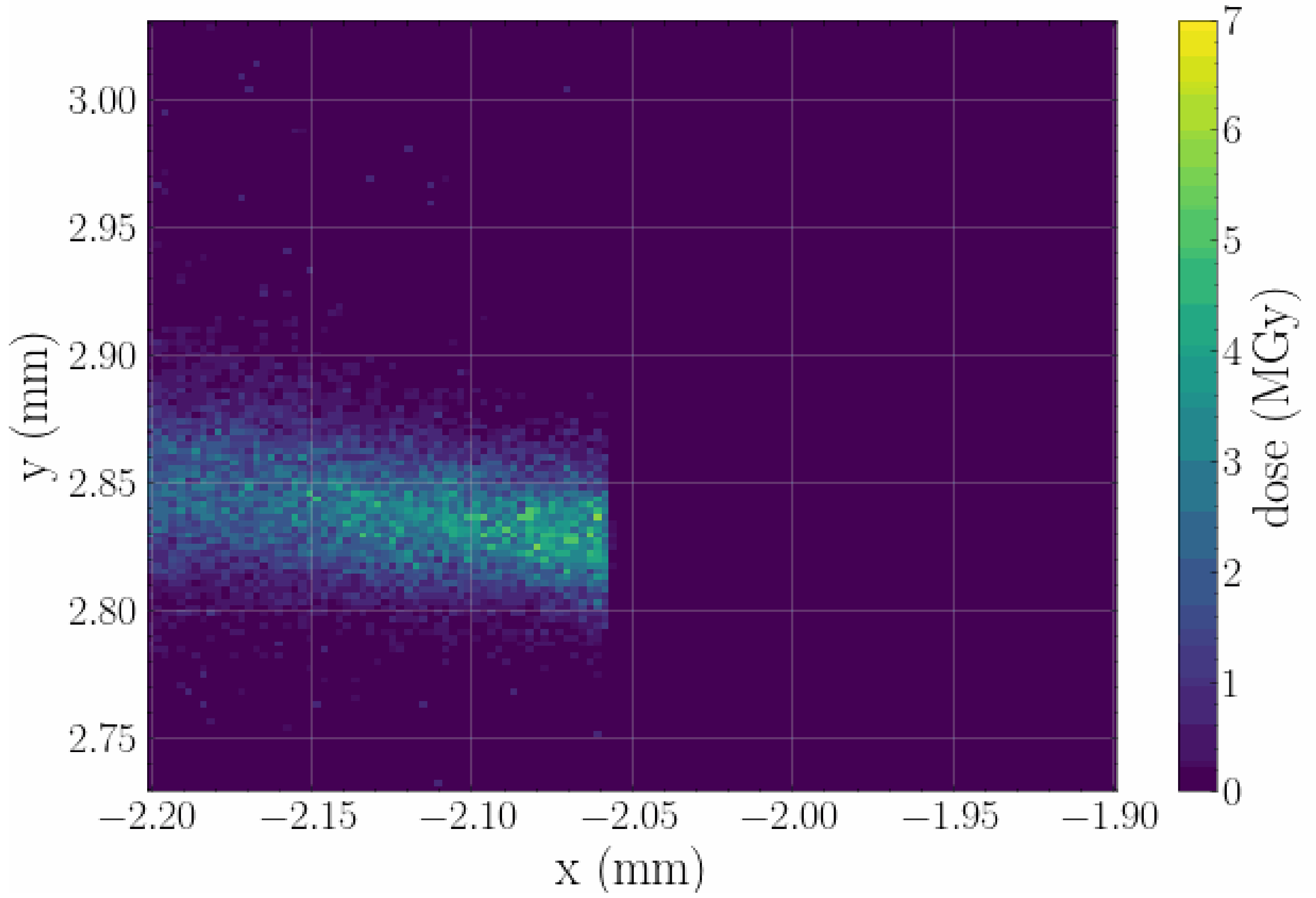


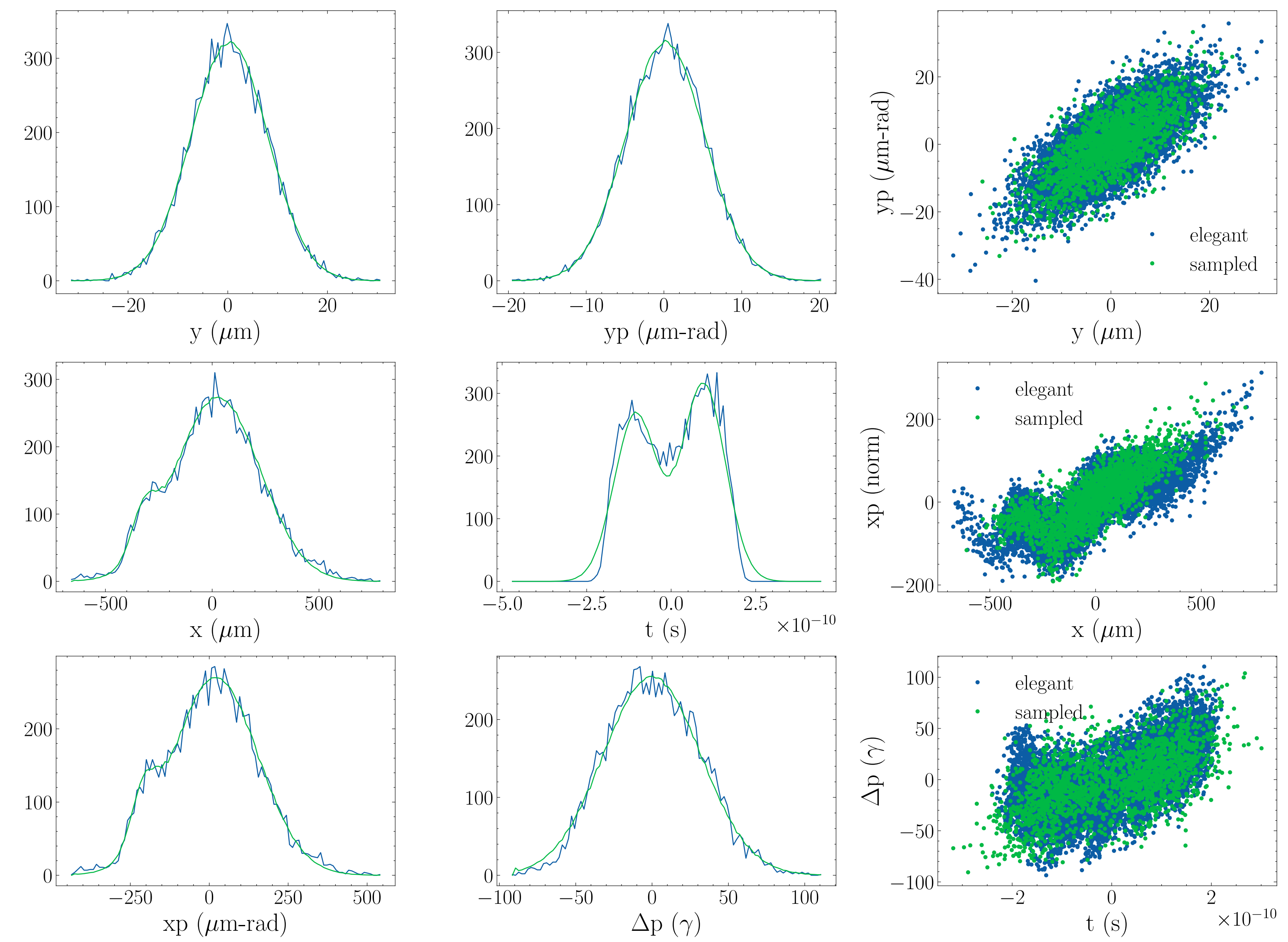
FLUKA permits accurate, adaptive dose calculations

- FLUKA is a general-purpose tool for particle transport and particle interaction with matter
  - Our use case: Monte Carlo calculations of electron and photon interactions across a broad energy range
    - Multiple Coloumb scattering, Bremmstrahlung, secondary photon interactions (pair production, scattering)
  - Sophisticated geometry support for representing complex structures
- Dosimetry calculations are sensitive to particle statistics and number of interaction cycles
  - Each Monte Carlo cycle is a significant increase in runtime and saturates at low particle counts
  - Sample distribution to increase particle count









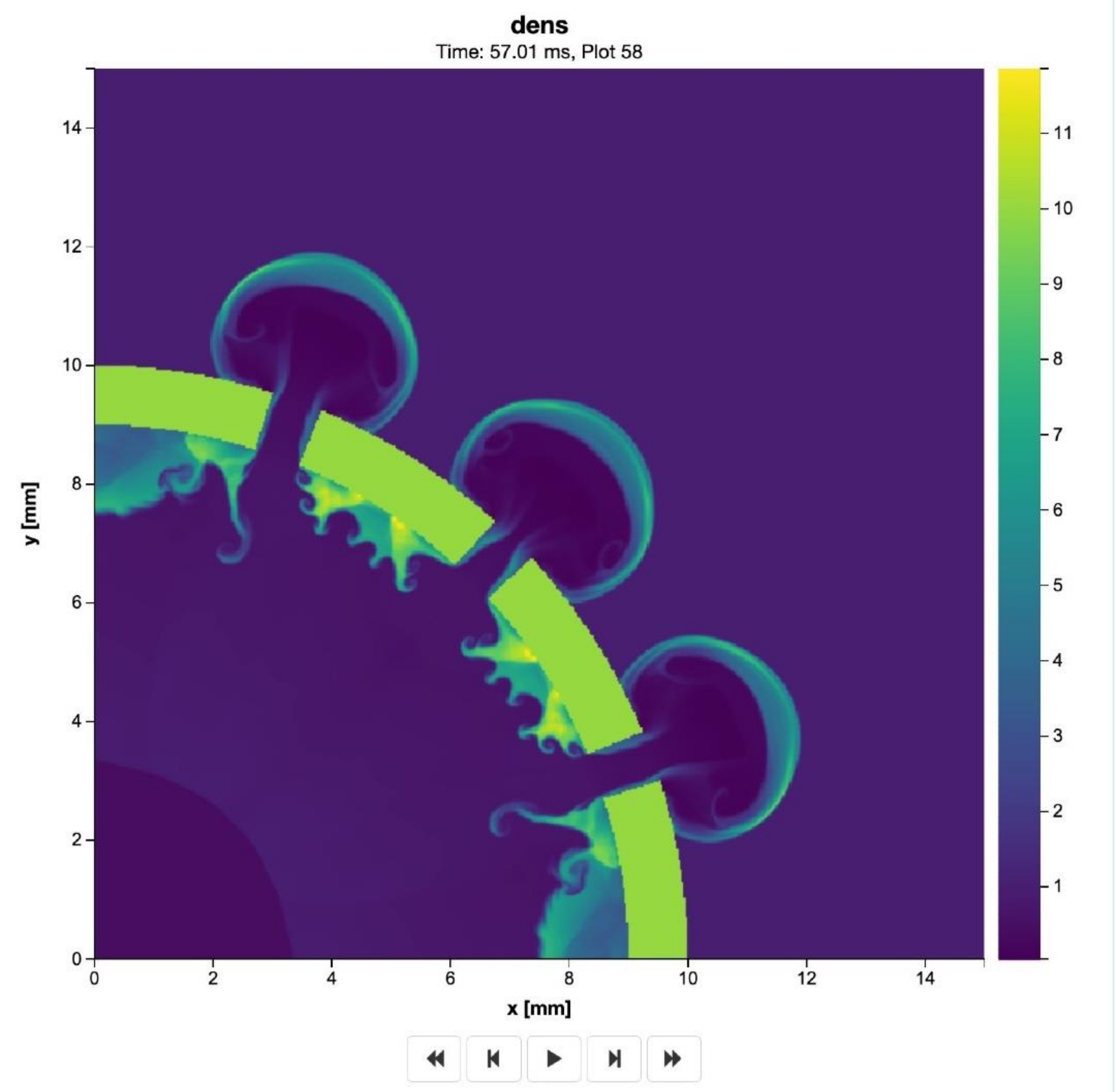
FLASH provides hydrodynamic response for a range of materials

- FLASH is a modular, multiphysics tool for radiation-hydrodynamics systems
    - Compressible flow evolution on a block-structured mesh with 3T representation of fluid (electron, ion, radiation)

$$\left\{\begin{array}{c}\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\boldsymbol{v})=0\\ \frac{\partial}{\partial t}(\rho\boldsymbol{v})+\nabla\cdot(\rho\boldsymbol{v}\boldsymbol{v})+\nabla P_{\mathrm{tot}}=0\\ \frac{\partial}{\partial t}(\rho E_{\mathrm{tot}})+\nabla\cdot[(\rho E_{\mathrm{tot}}+P_{\mathrm{tot}})\boldsymbol{v}]=Q_{\mathrm{las}}-\nabla\cdot\boldsymbol{q}\end{array}\right\}$$

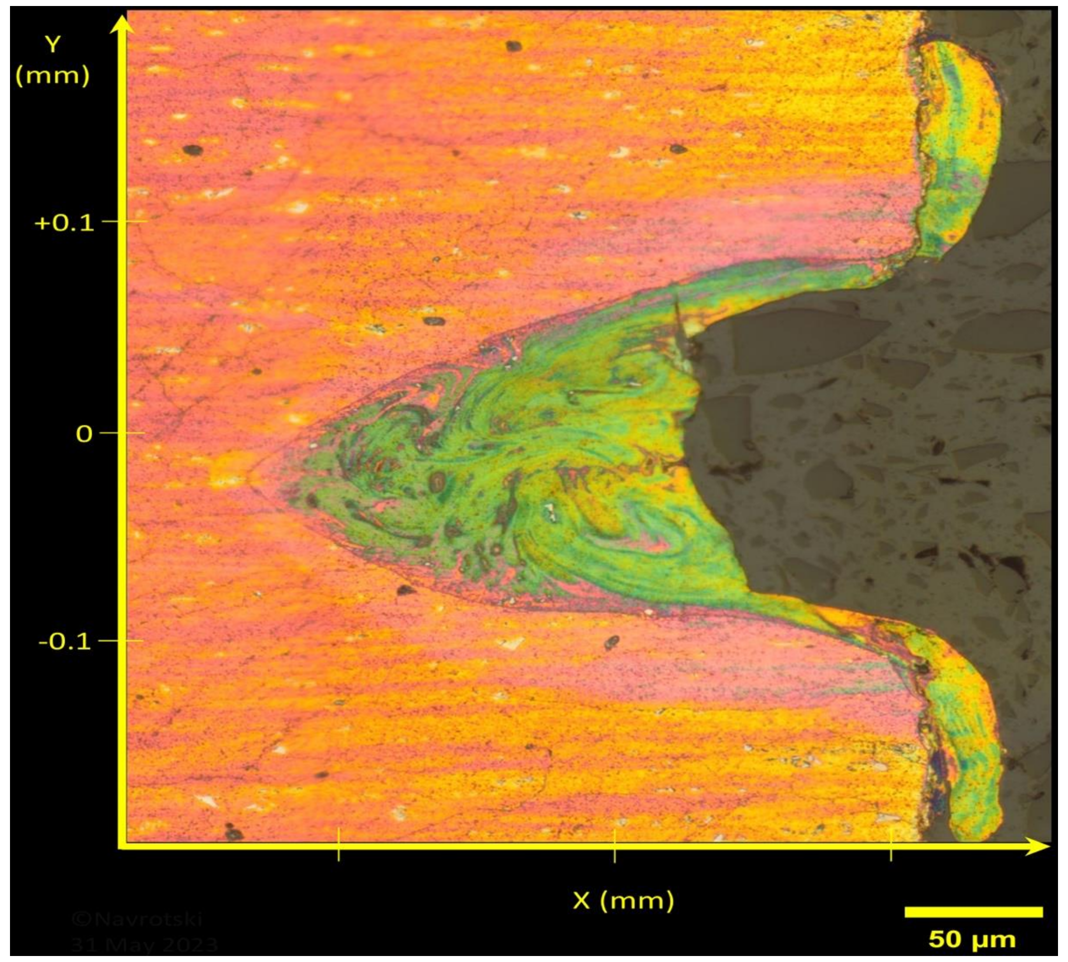
$$\left\{\begin{array}{c}\frac{\partial}{\partial t}(\rho e_{\mathrm{i}})+\nabla\cdot(\rho e_{\mathrm{i}}\boldsymbol{v})+P_{\mathrm{i}}\nabla\cdot\boldsymbol{v}=\rho\frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_{\mathrm{e}}-T_{\mathrm{i}})\\ \frac{\partial}{\partial t}(\rho e_{\mathrm{e}})+\nabla\cdot(\rho e_{\mathrm{e}}\boldsymbol{v})+P_{\mathrm{e}}\nabla\cdot\boldsymbol{v}=\rho\frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_{\mathrm{i}}-T_{\mathrm{e}})-\nabla\cdot\boldsymbol{q}_{\mathrm{e}}+Q_{\mathrm{abs}}-Q_{\mathrm{emis}}+Q_{\mathrm{las}}\\ \frac{\partial}{\partial t}(\rho e_{\mathrm{r}})+\nabla\cdot(\rho e_{\mathrm{r}}\boldsymbol{v})+P_{\mathrm{r}}\nabla\cdot\boldsymbol{v}=\nabla\cdot\boldsymbol{q}_{\mathrm{r}}-Q_{\mathrm{abs}}+Q_{\mathrm{emis}}\end{array}\right\}$$

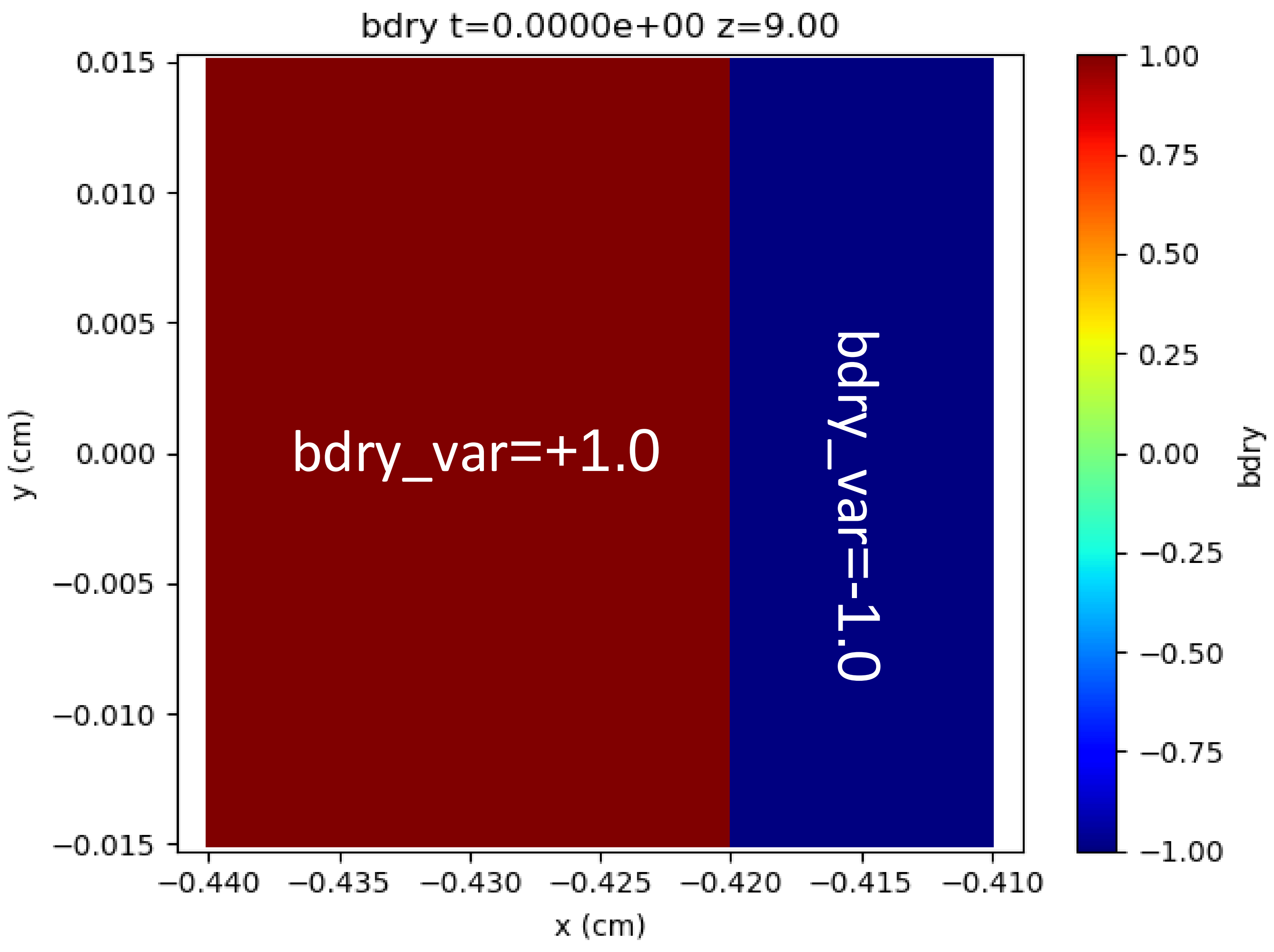
-
    - Magnetic field evaluation via unsplit, staggered mesh scheme
- Specific capabilities for laboratory and high energy density plasma systems:
    - Single fluid, multi-species description with adjustable compositions
    - Arbitrary specification of temperature, density profiles for initial conditions
    - Tabulated EOS for flexible internal energy, ionization, and opacity
    - Configurable time-dependent energy deposition from external sources
    - HPC capable – AMR, parallel I/O, scaling to 10s of thousands of cores (MPI)
    - openPMD support is in development for coupling to community PIC codes
- Accessible through download and through Sirepo app
    - http://flash.rochester.edu/
    - Try it out: https://www.sirepo.com/flash#/

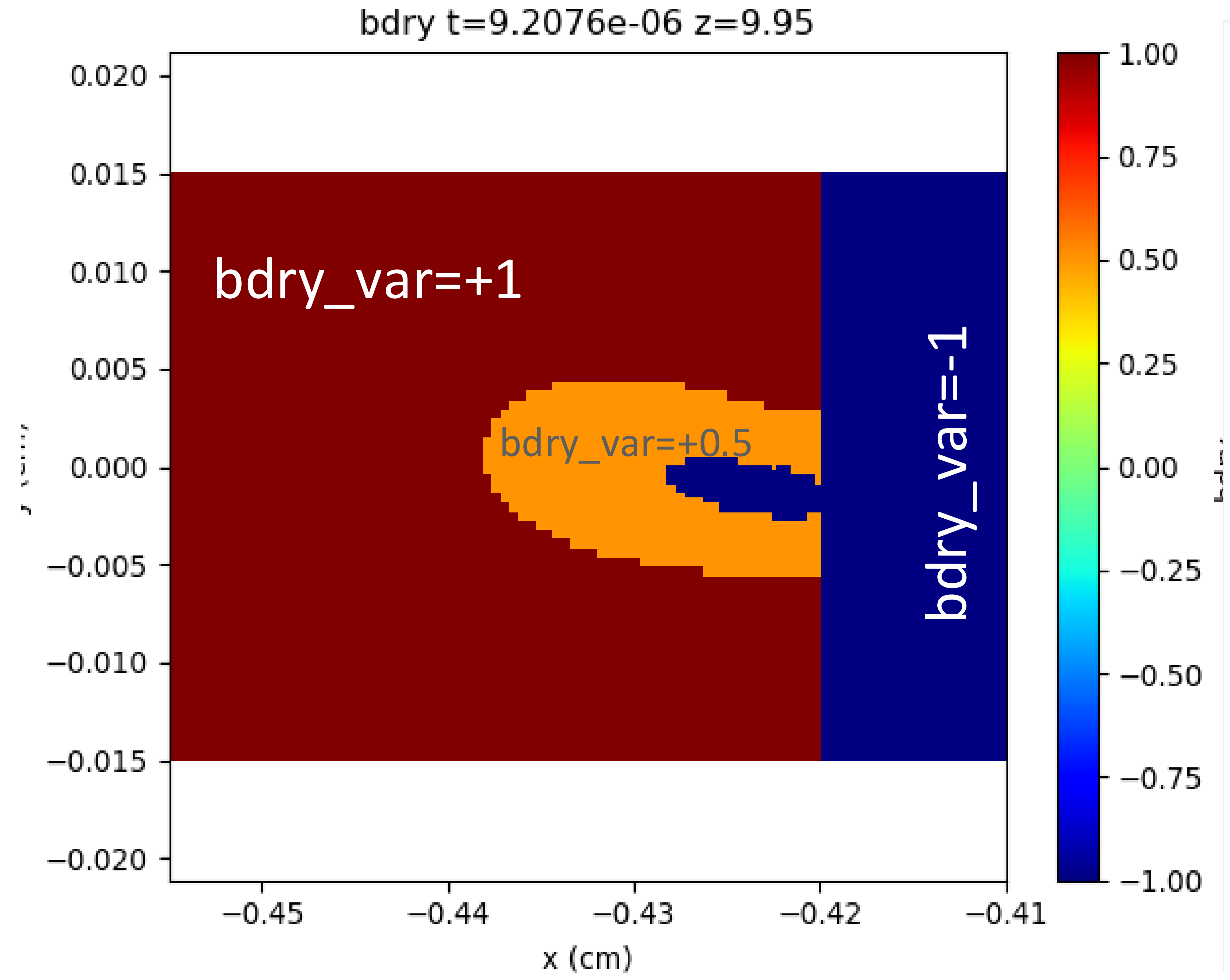


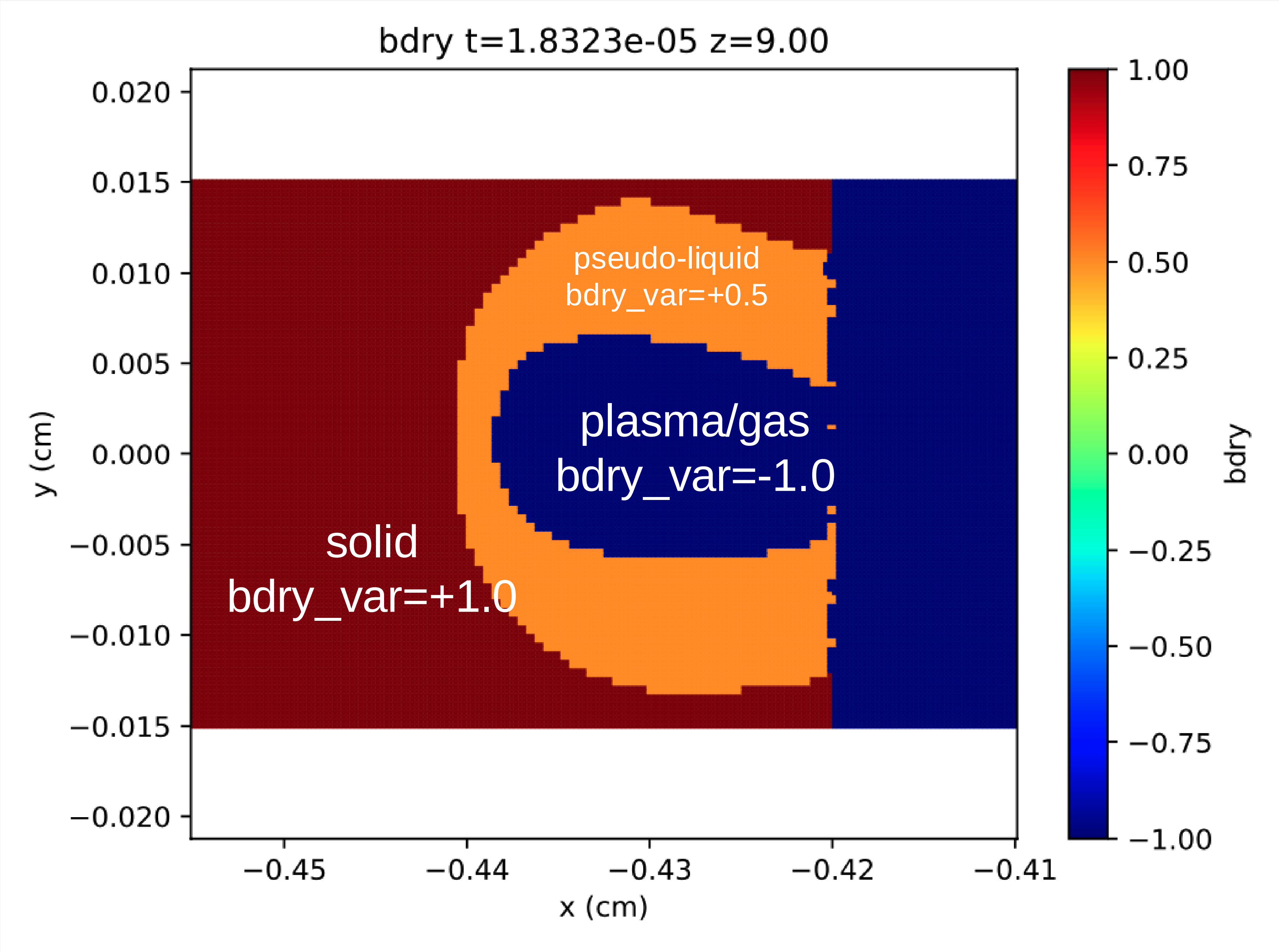
Collimator material shows evidence of phase change during beam strikes

- Experiments indicate melting and evaporation, and re-solidification
- Phase modeling in FLASH requires extrinsic support
  - Set `BDRY_VAR=+1.0` to fix cells as rigid
  - Set `BDRY_VAR=-1.0` to permit full hydrodynamics
- Modifications to permit intermediate phases
  - Set `BDRY_VAR=+0.5` to specify intermediate "pseudo-liquid" phase
    - Thermal conductivity modified in line with temperature/phase
    - Retains rigid body approximation (e.g. no advection)









Phase change necessitates improved transport properties (I)

- Improvement of thermal conductivity via phase change labeling
  - FLASH employs a Spitzer model for thermal/electrical/magnetic transport for plasmas
  - Implemented a model for thermal conductivity which gives κ as a function of T in solid copper and aluminum
  - Implemented a model for thermal conductivity in liquid copper and liquid aluminum

$$\kappa_{Cu}(T) = \begin{cases} \kappa_{solid,Cu}(T), & T < T_{m,Cu} = 1357.77\text{ K} \\ \kappa_{liquid,Cu}(T), & T_{m,Cu} = 1357.77\text{ K} \le T \le T_{b,Cu} = 2835\text{ K} \end{cases}$$

$$\kappa_{Al}(T) = \begin{cases} \kappa_{solid,Al}(T), & T < T_{m,Al} = 933.47\text{ K} \\ \kappa_{liquid,Al}(T), & T_{m,Al} = 933.47\text{ K} \le T \le T_{b,Al} = 2743\text{ K} \end{cases}$$

$$\kappa_{solid}(T) = (w_0 + w_i + w_{i0})^{-1} \quad \begin{cases} w_0 = \frac{\rho_i(273)}{(RRR-1)L_0 T} \\ w_i = \frac{P_1 T^{P_2}}{1+P_1 P_3 T^{(P_2+P_4)} \exp(-(P_5/T)^{P_6})} + w_c(T) \\ w_{i0} = \frac{P_7 w_i w_0}{w_i + w_0} \end{cases}$$

$$\begin{aligned} w_c(T) =& a_1 \ln\left(\frac{T}{b_1}\right) \exp\left[-\left(\frac{\ln(T/c_1)}{d_1}\right)^2\right] \\ &+ k a_2 \ln\left(\frac{T}{b_2}\right) \exp\left[-\left(\frac{\ln(T/c_2)}{d_2}\right)^2\right] \\ &+ a_3 \ln\left(\frac{T}{b_3}\right) \exp\left[-\left(\frac{\ln(T/c_3)}{d_3}\right)^2\right]. \end{aligned}$$

Hust, J. and Lankford, NBS IR 84-3007(1984) https://doi.org/10.6028/NBS.IR.84-3007

$$\kappa_{\text{liquid},Cu}(T) = c_1 + c_2(T - T_{m,Cu})$$

Assael *et al.*, High Temp High Press. 46(6):391-416. (2017)

$$\kappa_{\text{liquid},Al}(T) = a + bT + cT^2$$

Leitner *et al.*, *Metall Mater Trans A* **48**, 3036–3045 (2017) https://doi.org/10.1007/s11661-017-4053-6

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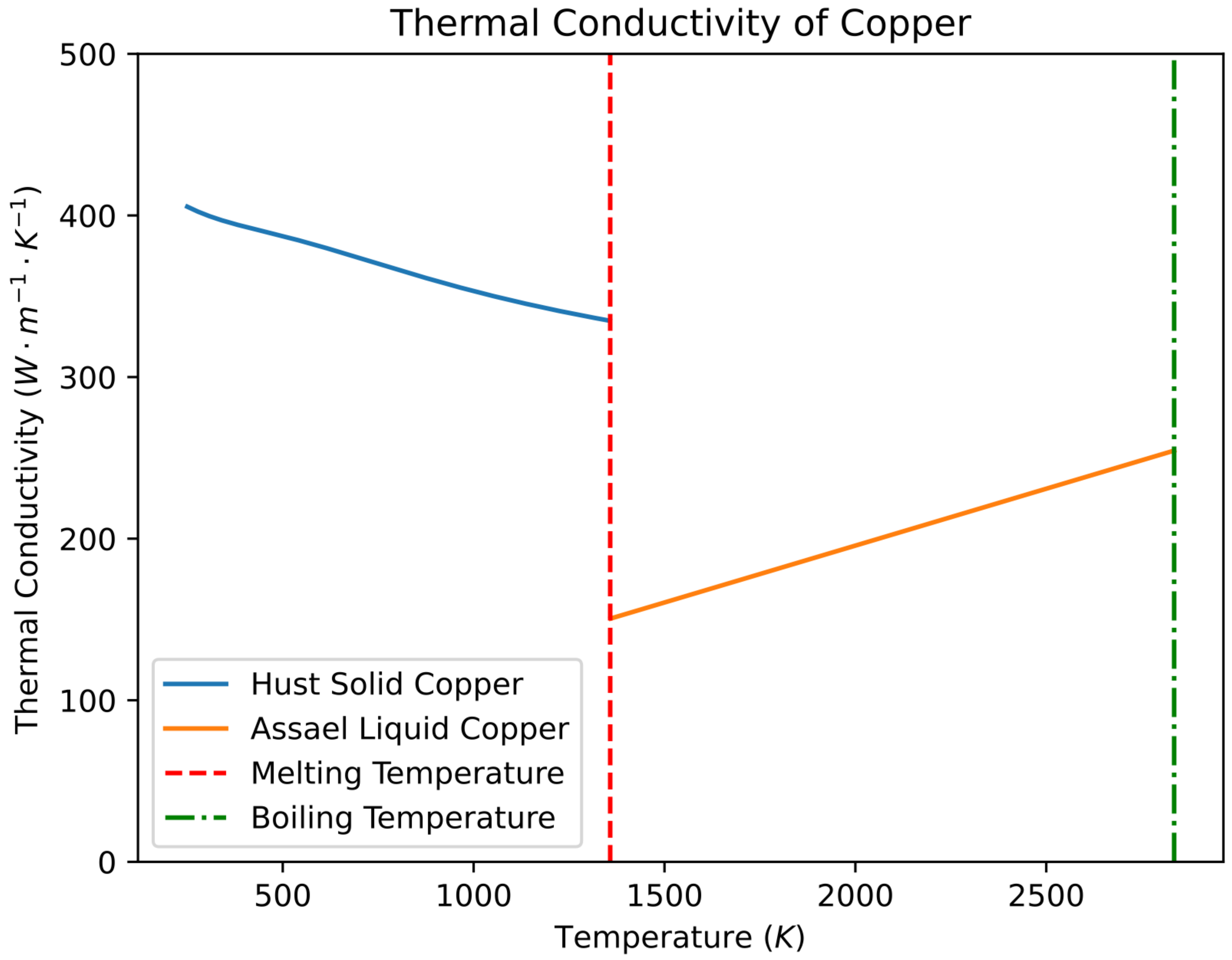
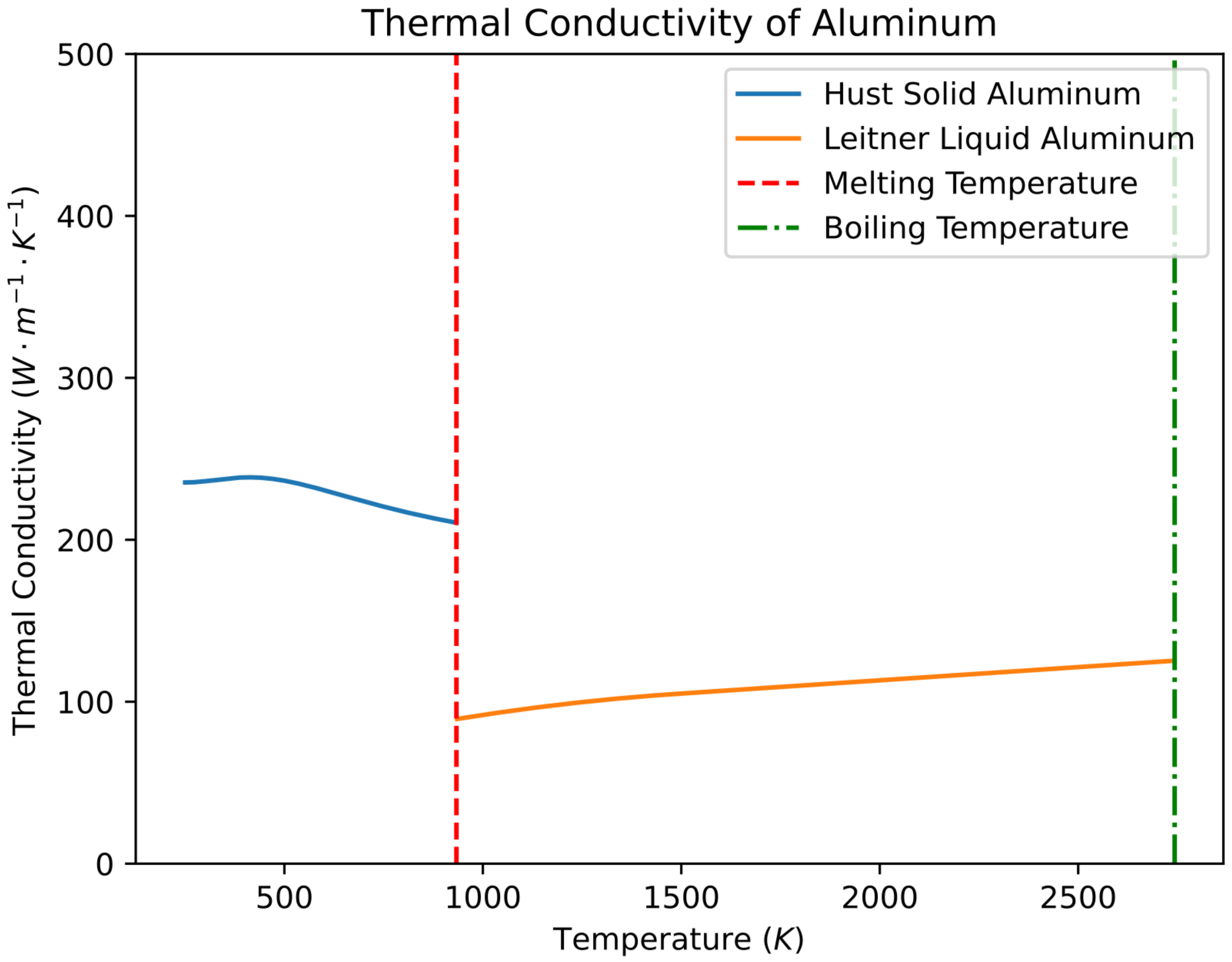
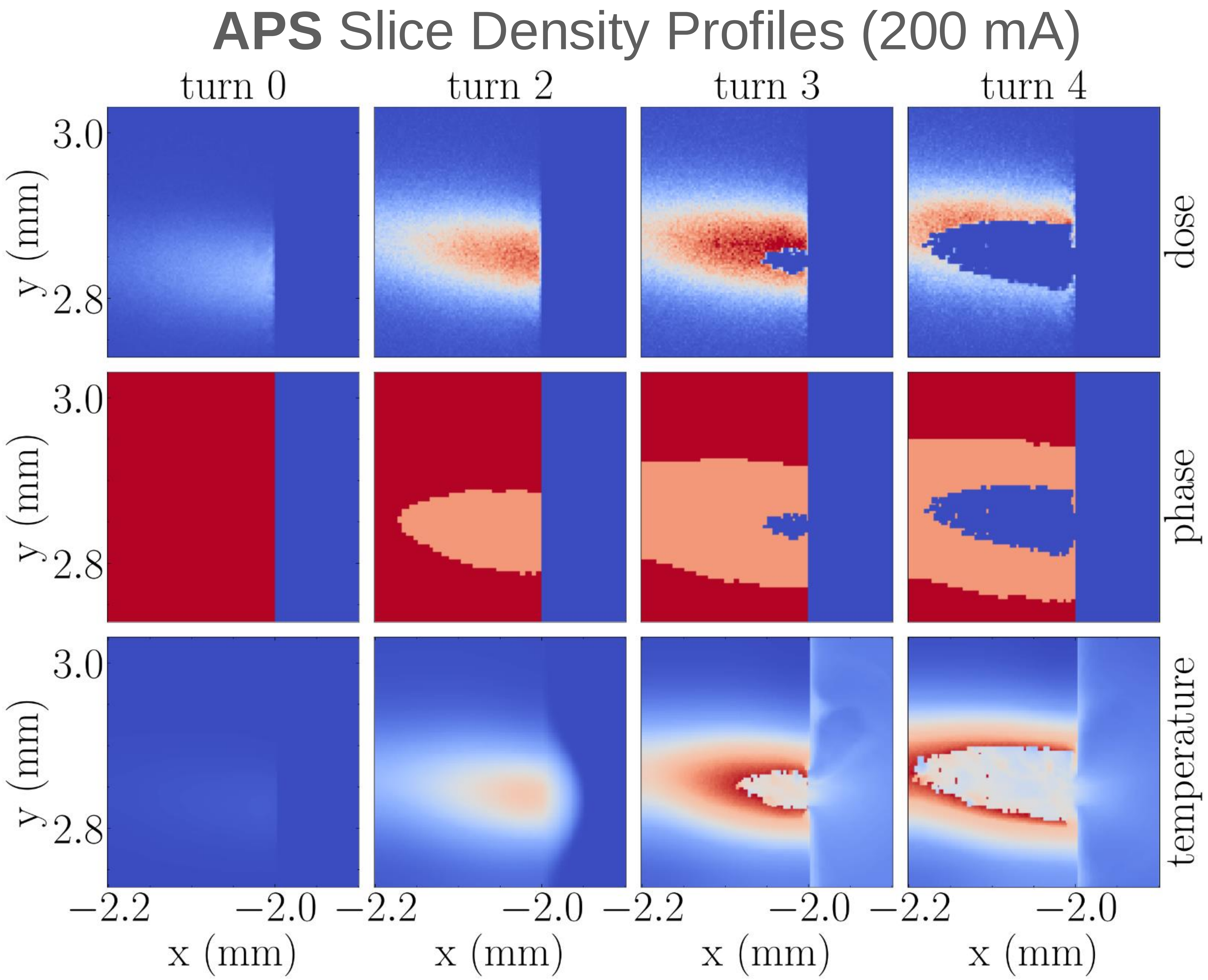
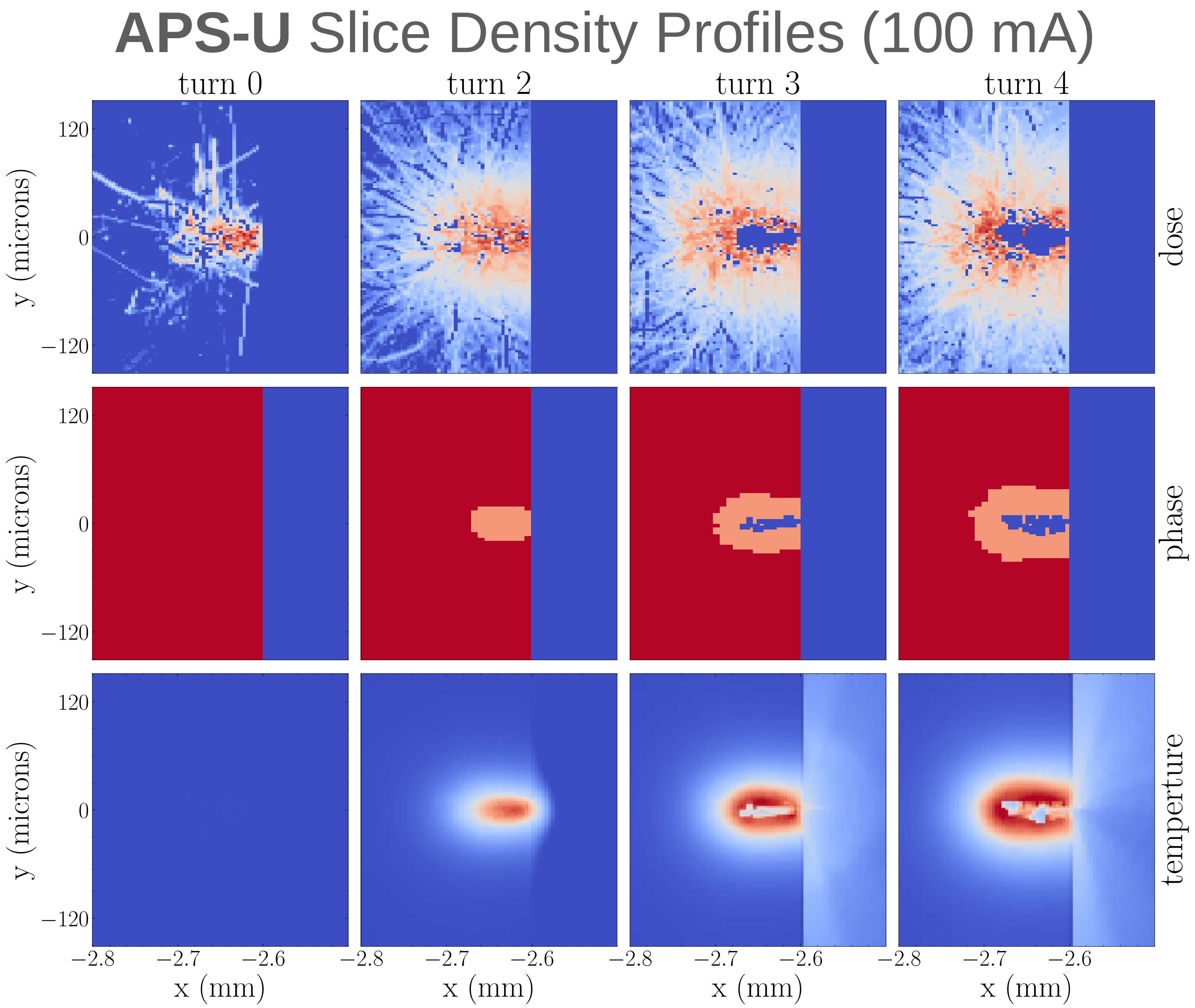




Coupled Simulations Indicate variation in response to bunch pattern

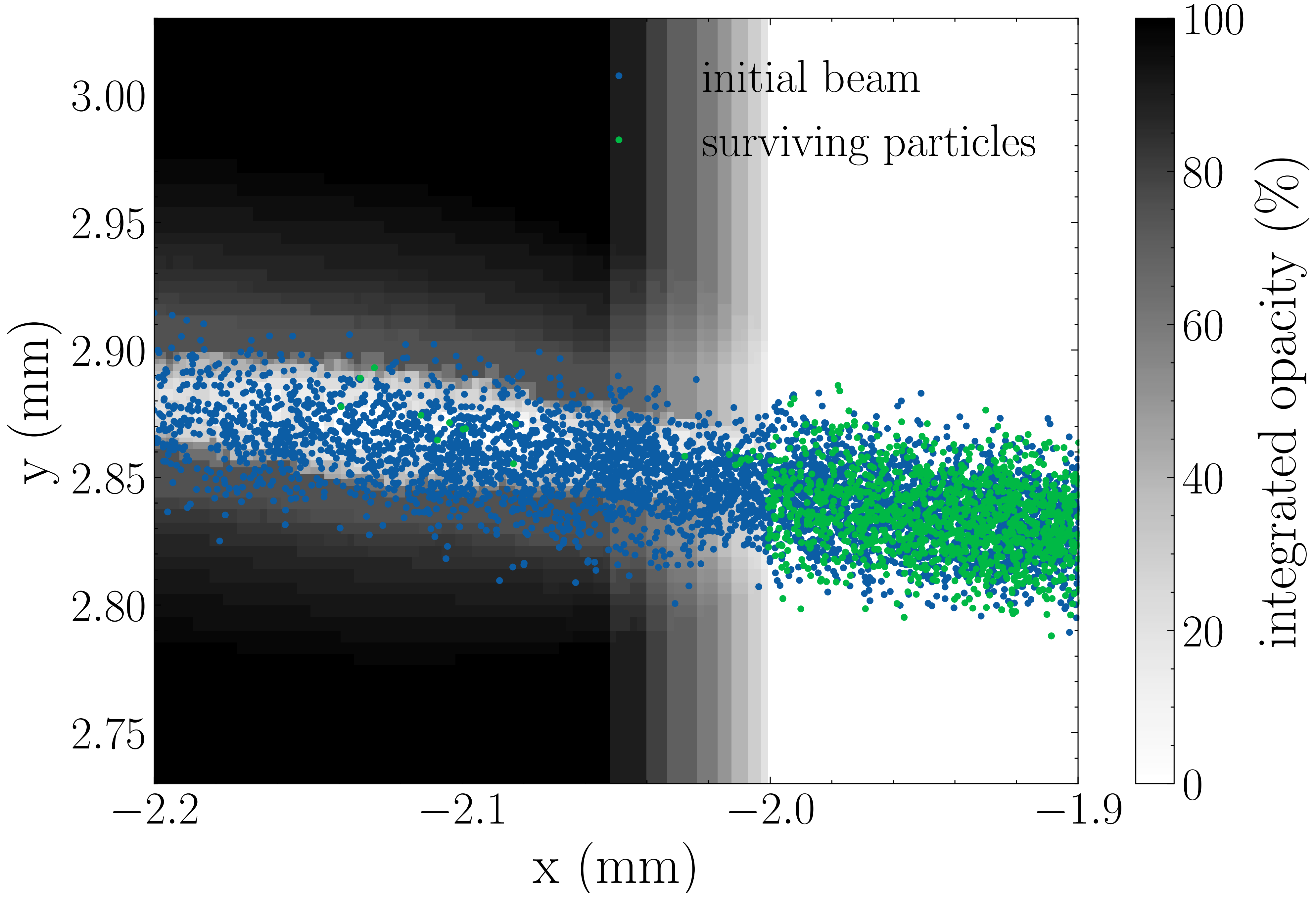
- Coupled simulations with a copper collimator illustration variation in APS and APS-U response
    - Larger APS beam features a higher current a more frequent bunch pattern
    - APS-U beam features a lower current with significantly smaller extent and narrower loss profile

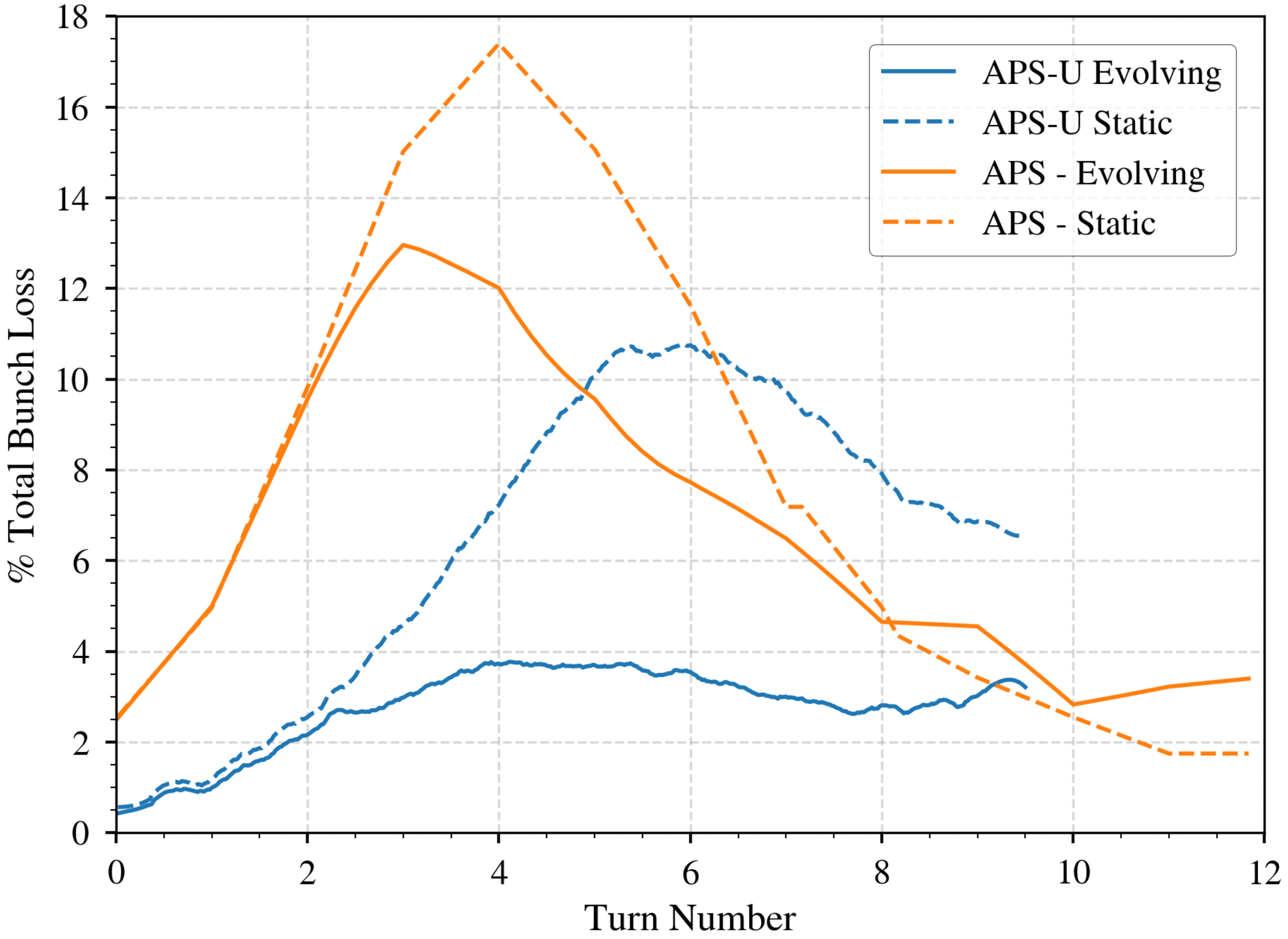

APS Slice Density Profiles (200 mA)


APS-U Slice Density Profiles (100 mA)

Proper coupling increases interaction length while reducing peak beam loss rates

- Multiple factors mitigate beam loss as a function time
  - Melt conditions and subsequent advection reduce density and therefore mitigate scattering and deposition
    - Cumulative losses are 15% lower by 12th turn
  - Reduced scattering limits peak beam loss and results in larger losses at high pass numbers
  - APS-U conditions are subject to reduced peak but more prolong losses in both cases
    - The bunch patterns and dynamics under RF abort differ significantly between the two machines

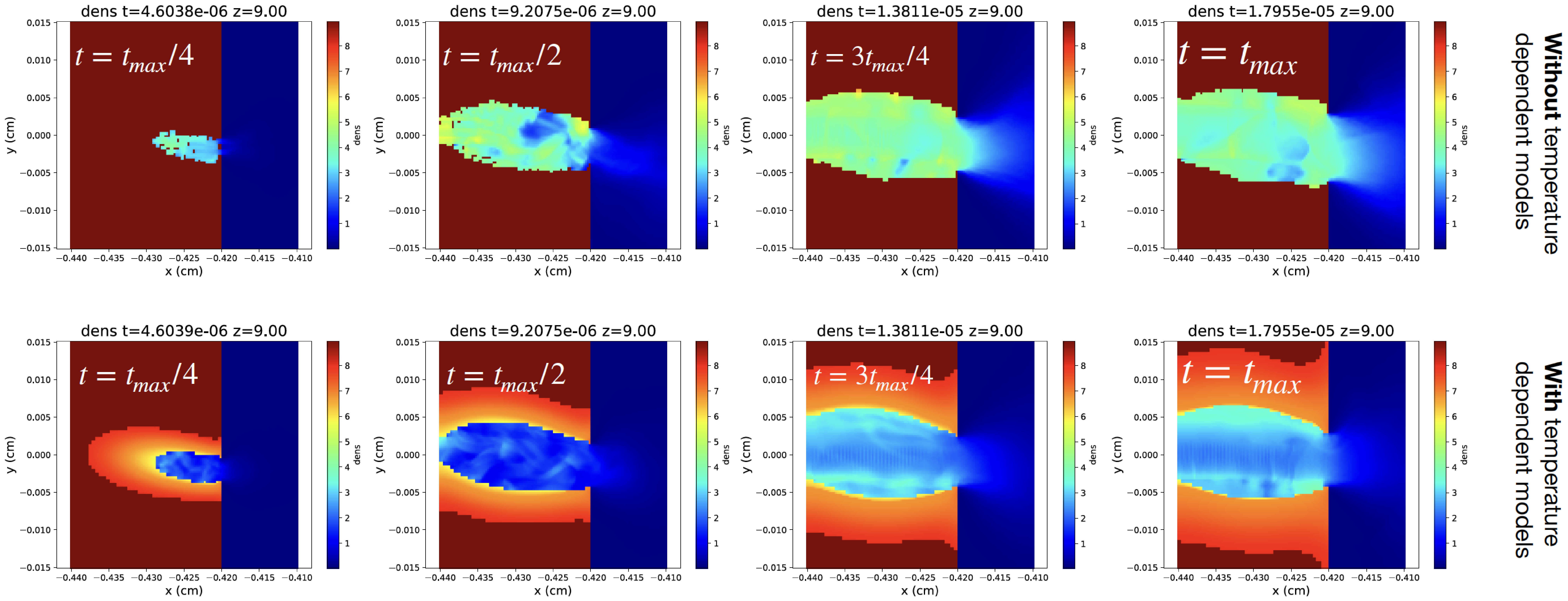




Choice of collimator material affects performance

- Moving from Copper to Aluminum can reduce structural damage
  - Damage is largely a function of density, which directly correlates to dose
  - Thermal conductivity and melting point matter too, but those vary much less than density
  - *Uncoupled* simulation results indicate the strong influence of material choice

Copper Slice Density Profiles



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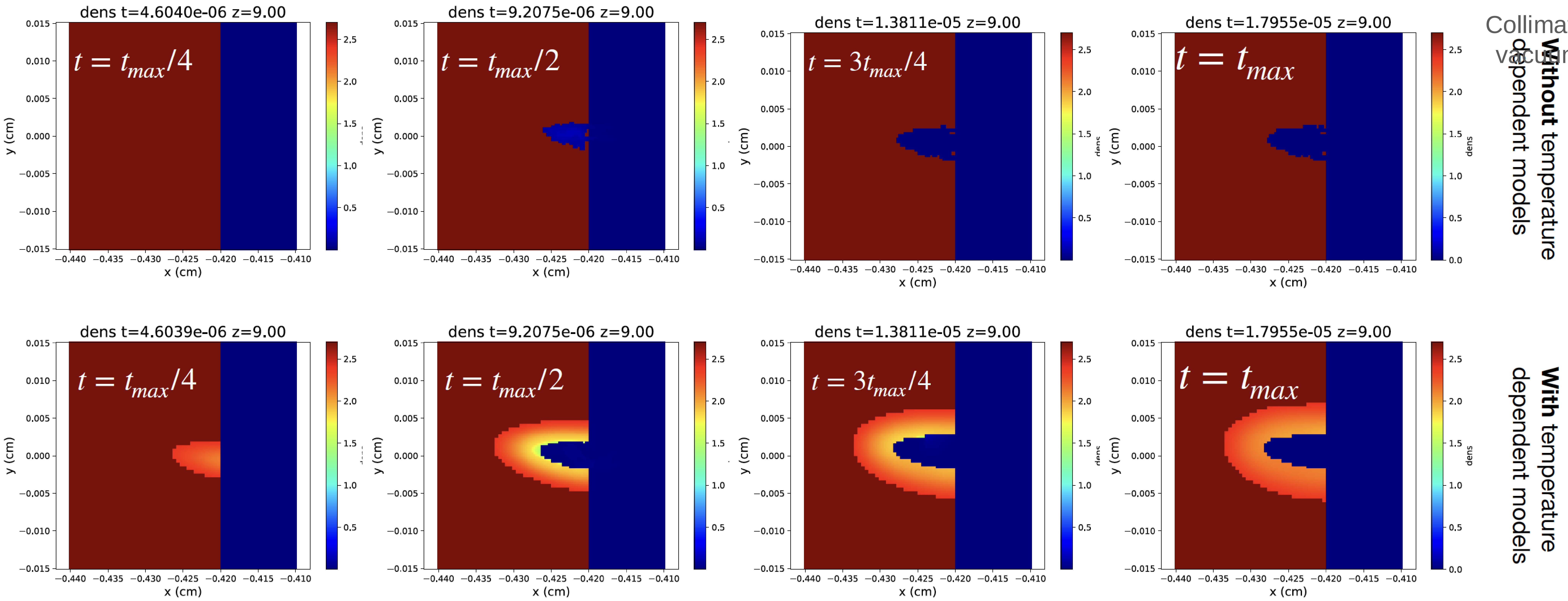
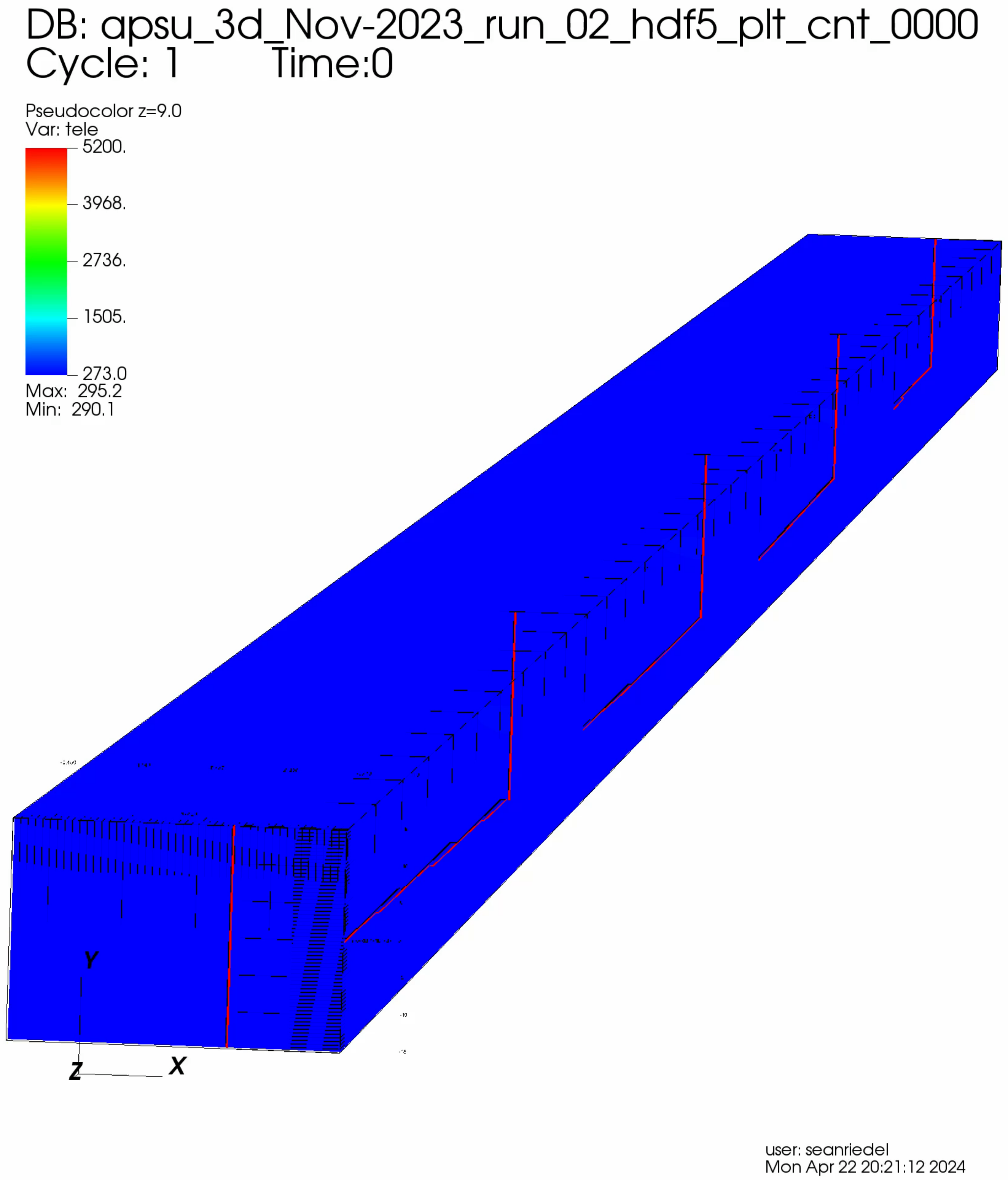
Aluminum Slice Density Profiles

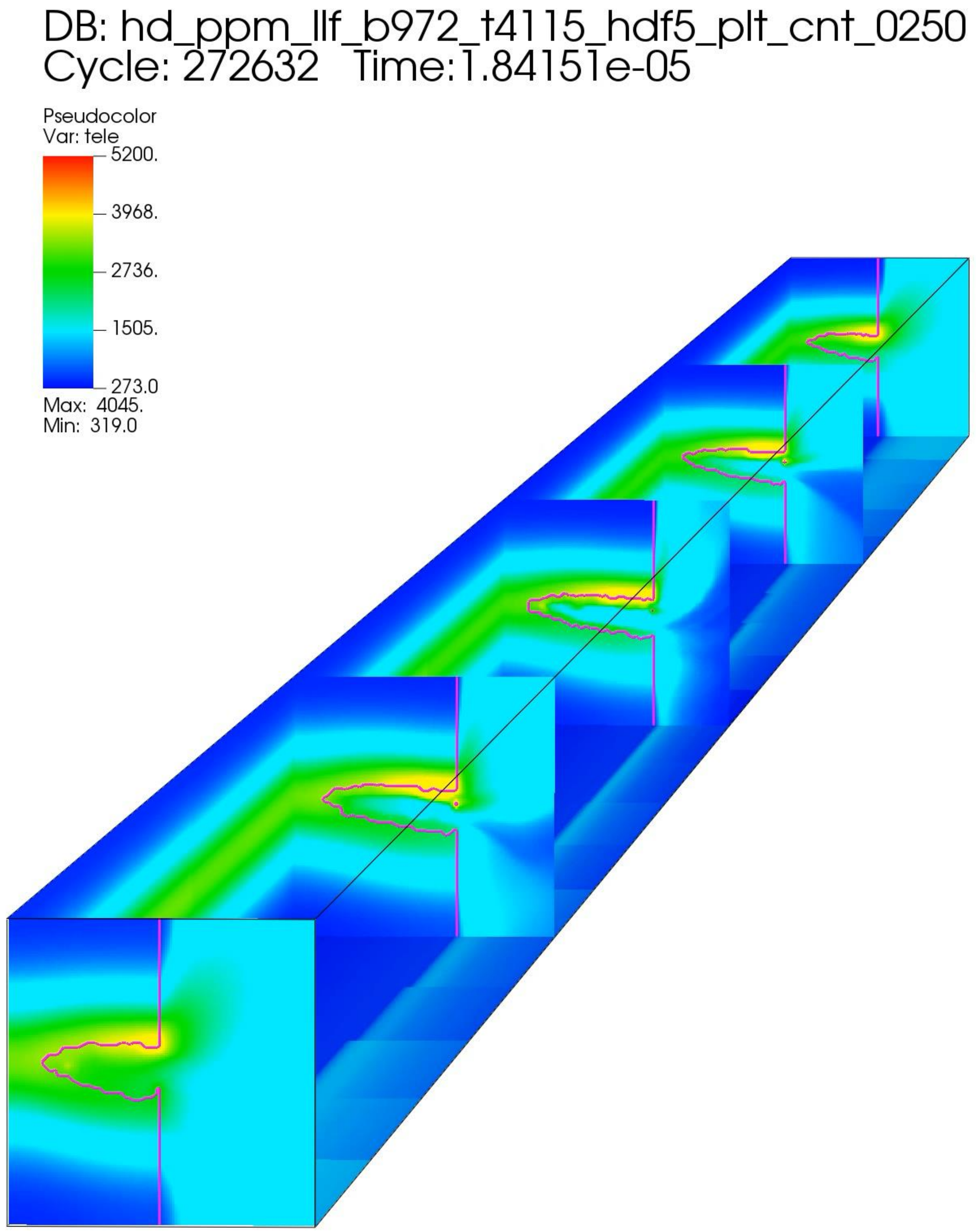


Collimator inside of vacuum chamber

Three-Dimensional modeling captures longitudinal collimator variation

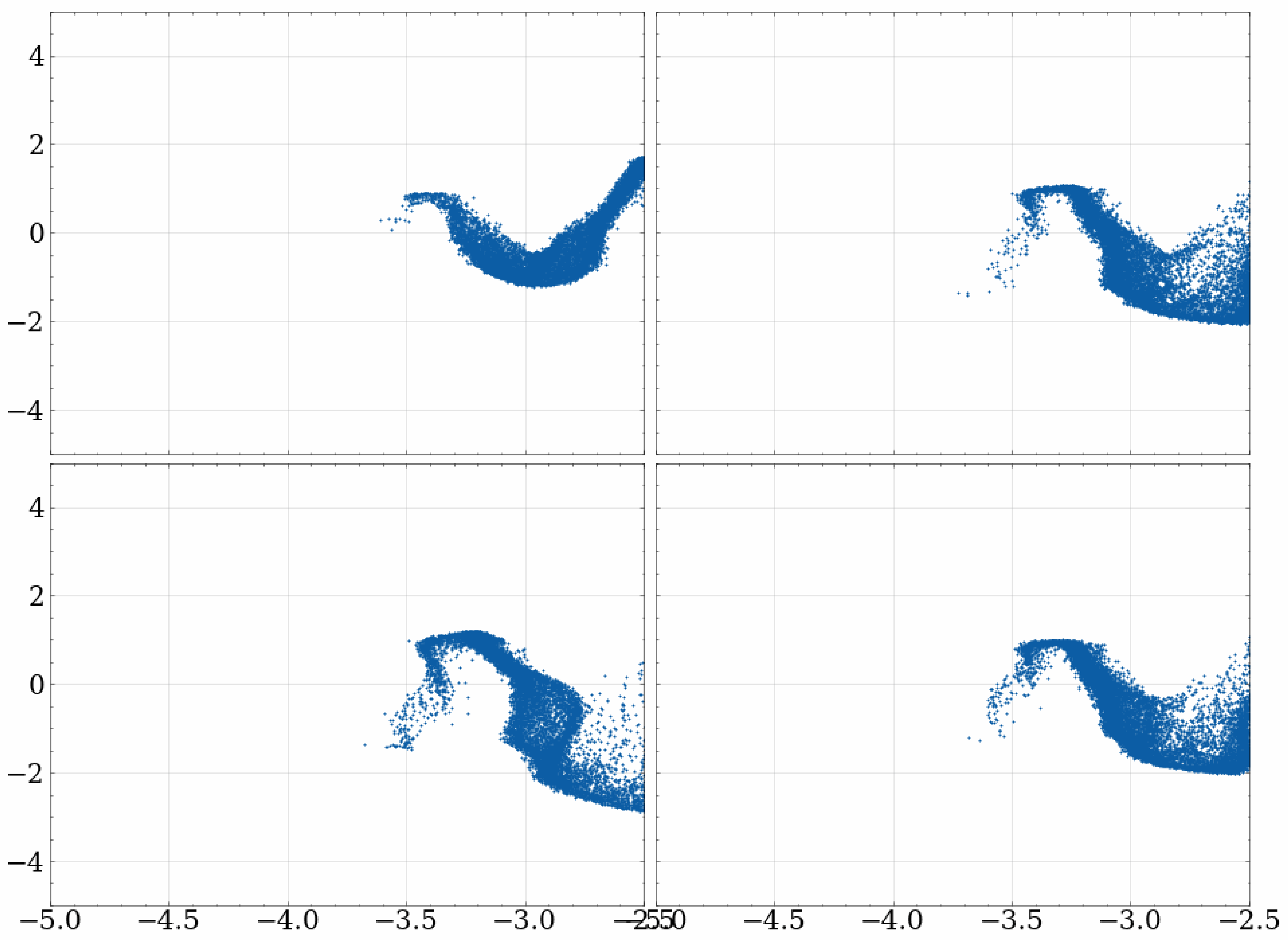
- Collimator arc increases deposition and damage at midpoint, subject to scattering effects

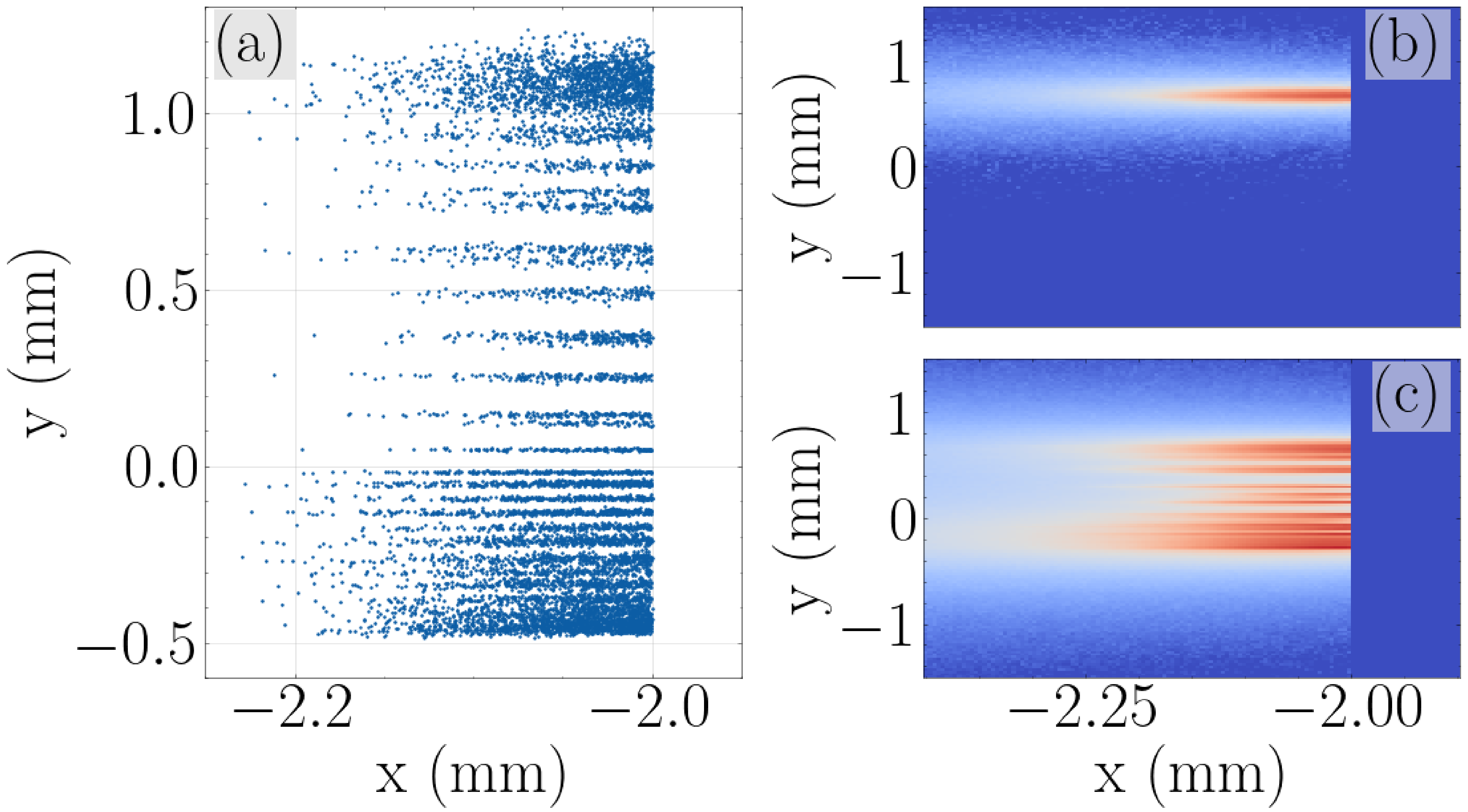




Fan-out kicker may mitigate damage to the collimator target

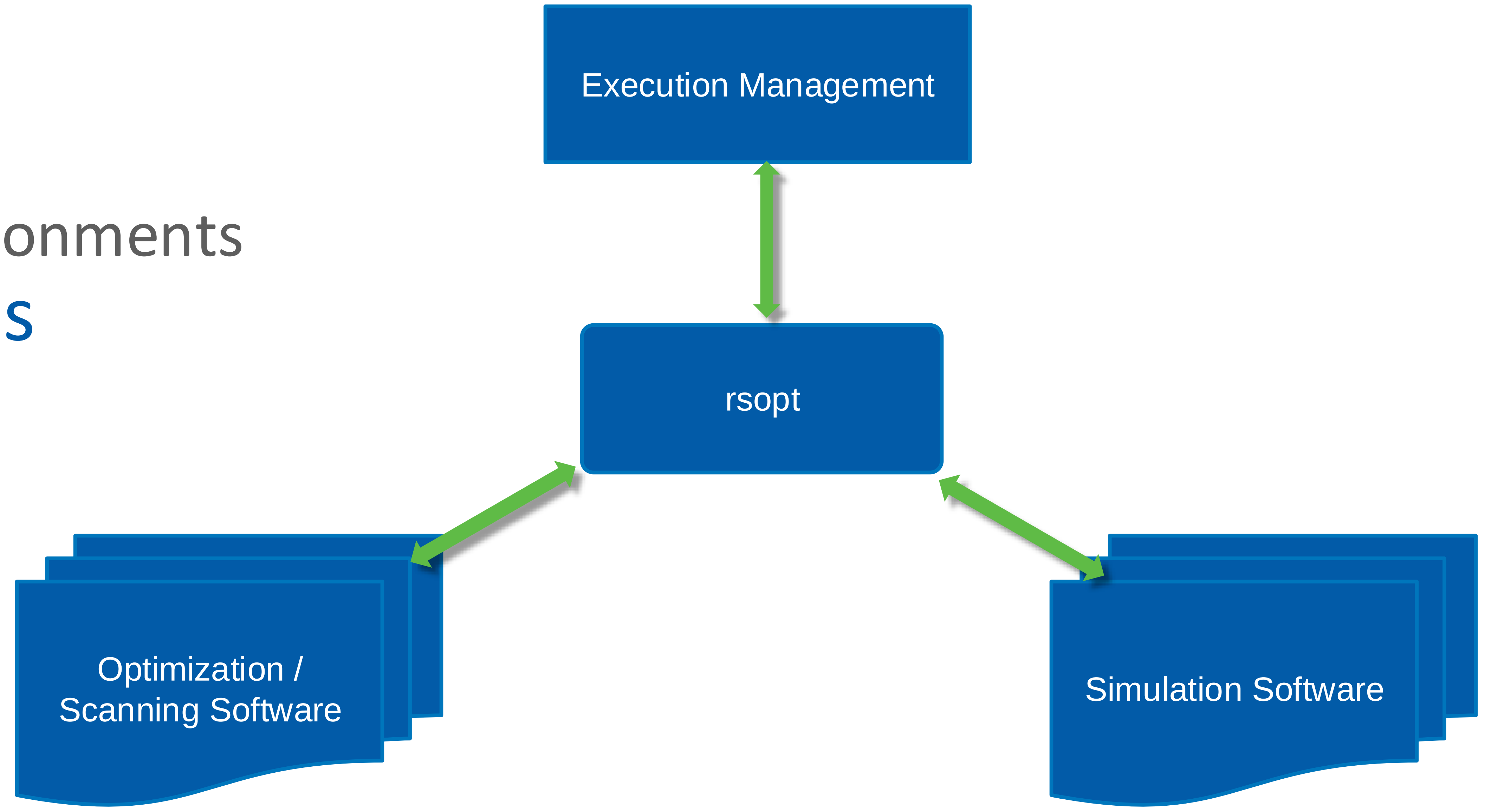
- Experiments have studied damage mitigation via the use of a vertically deflecting fan-out kicker (FOK) that spreads the bunch train transversely across the target
  - The FOK operates across individual bunches to spread them transversely and reduce incident power
  - Each bunch strikes the collimator in different vertical positions, stratifying the per-turn dose
  - Experiments indicate that the FOK is a powerful tool for damage mitigation
  - Initial models have been implemented to capture the bunch separation and transverse spread
    - These simulations indicate qualitative agreement with the reduction in dose





Improving simulation coordination to support multi-code workflow (I)

- Plan to leverage `rsopt` library to mediate simulations on distributed resources
  - Creates and manages simulation jobs and workers to perform complex ensembles of simulations from templated inputs
  - Leverages optimization libraries and/or custom procedures to generate simulation parameters
  - Easily transfer workflows from local machines onto HPC environments
- Growing support for start-to-end simulation modalities
  - Multiple codes with I/O handoffs supported for some common accelerator codes & Python scripting



- Supported codes
  - elegant*
  - MAD-X*
  - OPAL*
  - FLASH*
  - Genesis*
  - Python
  - User supplied

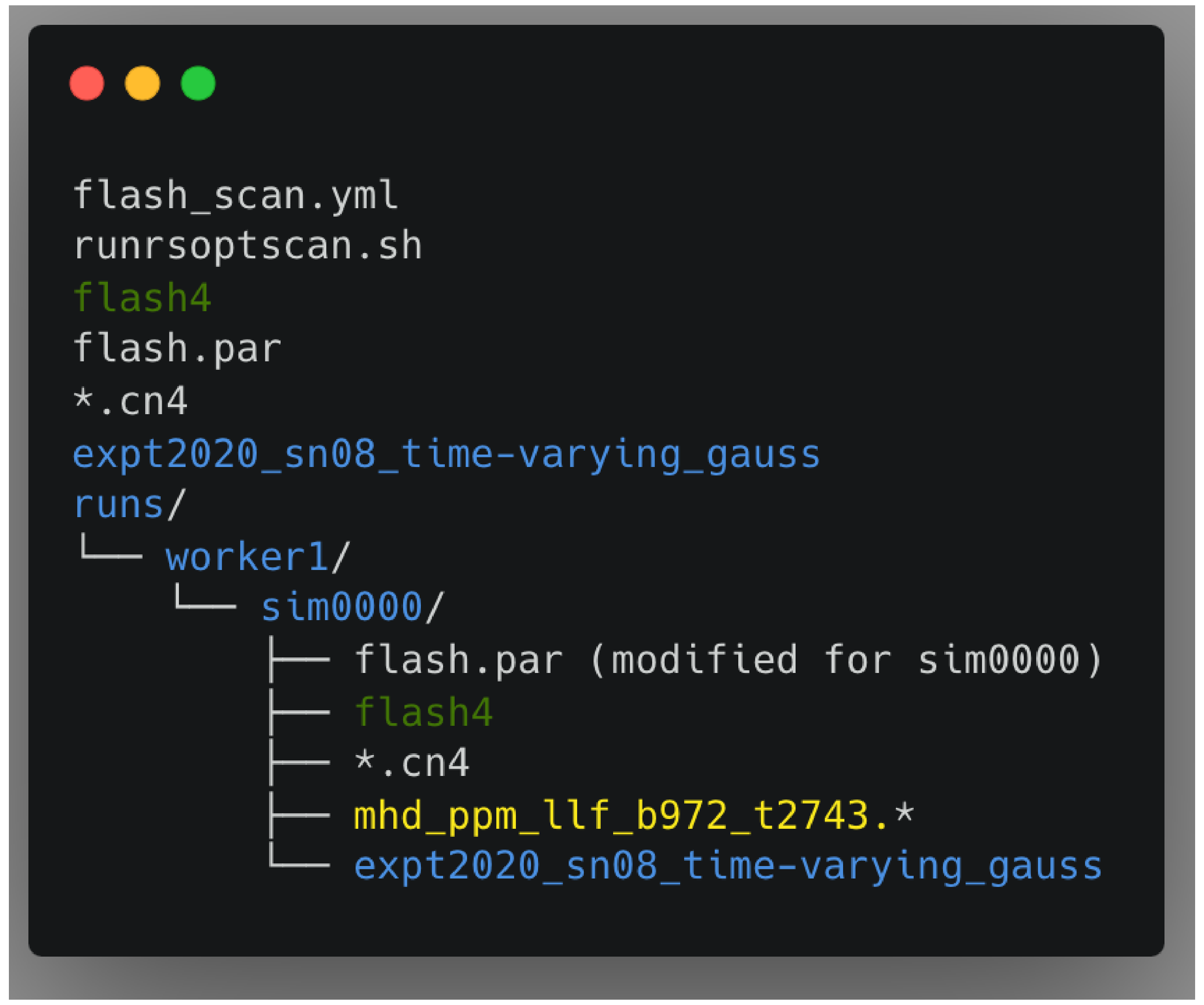
- Execution methods
  - serial
  - parallel (MPI)
  - Podman/Shifter (NERSC)

https://github.com/radiasoft/rsopt

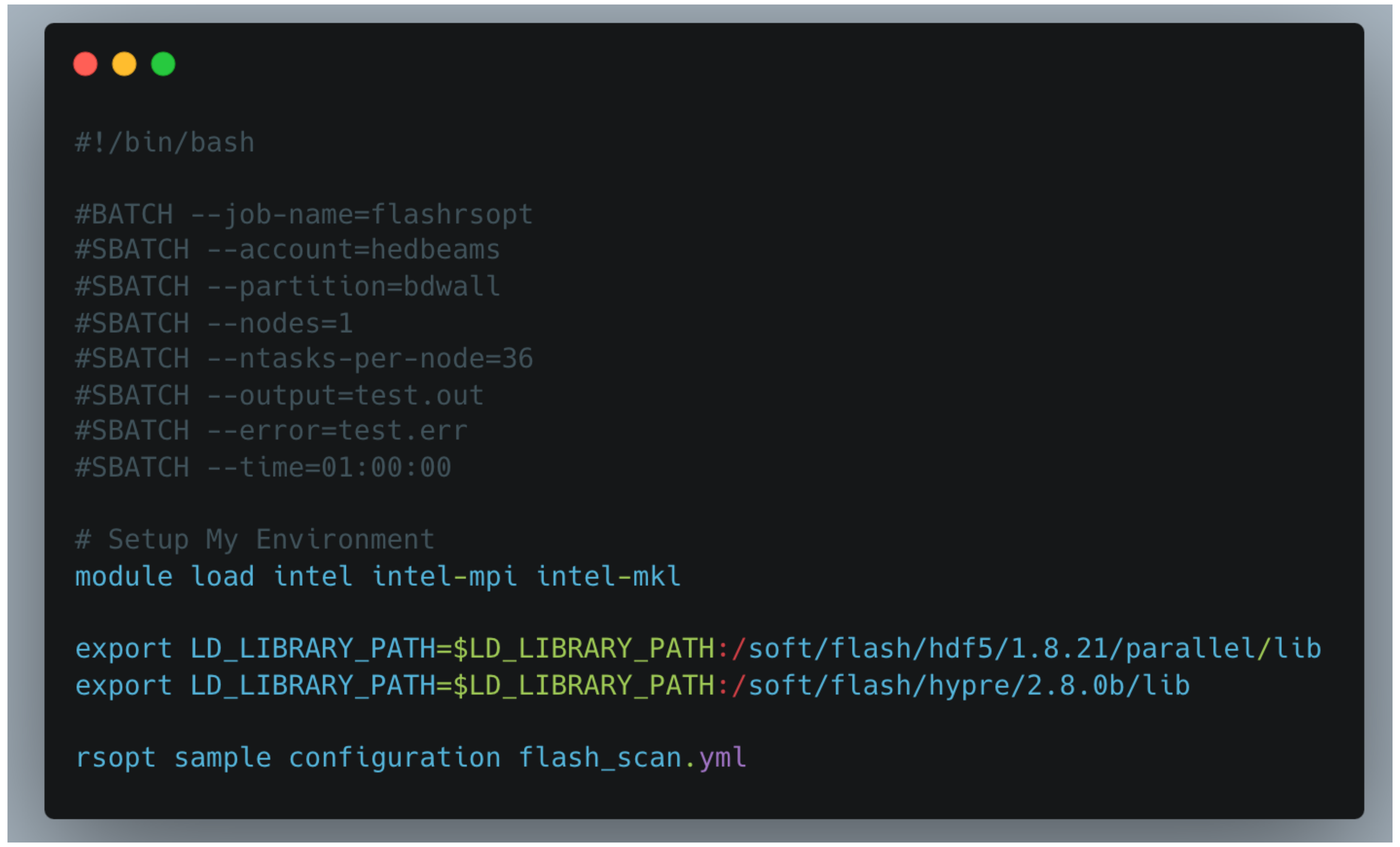
*File parsing supported

Simulation coordination to support multi-code workflow (II)

- Example demonstration with a simple parameter scan
  - Vary arbitrary parameters using `mesh_scan` mode
    - Latin Hypercube Sampling in parameters – supports arbitrary parametric variations with arbitrary sample number
  - External files identified and copied to run directory during execution
    - Supports folders with recursive file structure (e.g. deposition)
- Resulting file structure is recursive by worker/job
  - Analysis scales to many cores/workers
- Multi-code modeling links different configurations together
  - Support for arbitrary executables across all applications
  - Pre-compiled executables can be adopted via `user’ code approach



```
flash_scan.yml
runrsoptscan.sh
flash4
flash.par
*.cn4
expt2020_sn08_time-varying_gauss
runs/
└── worker1/
    └── sim0000/
        ├── flash.par (modified for sim0000)
        ├── flash4
        ├── *.cn4
        ├── mhd_ppm_llf_b972_t2743.*
        └── expt2020_sn08_time-varying_gauss
```



```
#!/bin/bash

#BATCH --job-name=flashrsopt
#SBATCH --account=hedbeams
#SBATCH --partition=bdwall
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=36
#SBATCH --output=test.out
#SBATCH --error=test.err
#SBATCH --time=01:00:00

# Setup My Environment
module load intel intel-mpi intel-mkl

export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/soft/flash/hdf5/1.8.21/parallel/lib
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/soft/flash/hypre/2.8.0b/lib

rsopt sample configuration flash_scan.yml
```

```
codes:
    - flash:
        settings:
        parameters:
            sim_rhoAmbient:
                min: 1.673e-6
                max: 6.695e-6
                start: 1.673e-6
                samples: 8
        setup:
            input_file: flash.par
            executable: flash4
            execution_type: parallel
            cores: 36
    - python:
        settings:
            macroparticle_count: 32_000
        parameters:
            paramater_a:
                min: 42.0
                max: 84.0
                start: 64.0
                samples: 3
        setup:
            preprocess: ["process.py",
"create_warpx_input"]
            input_file: run_warpx.py
            function: main
            execution_type: parallel
            cores: 128
options:
    run_dir: ./runs
    software: mesh_scan
    sym_links:
        - h2_fill.cn4
        - "Bessel_temp_files/"
```

Conclusions & Next Steps

- Next generation light sources face machine protection challenges from high brightness beams
  - Full beam aborts threaten destruction of collimators responsible from protecting critical insertion devices
- Coupled workflow enables self-consistent simulations of beam and collimator interaction
  - Combination of beam dynamics, particle-matter interaction, and material hydrodynamics
- Existing models show promise in capturing basic responses under APS and APS-U conditions
  - Models provide guidance on mitigation efforts via material choice and fast beam expansion
- Next Steps will enhance physics, numerics, and workflow capabilities
  - *Extend intermediate phase conditions*
    - Include latent heat model and enable density and/or EOS modulations for intermediate phases
  - *Improve boundary conditions for mixed phase interactions*
    - Implement an immersed boundary method (IBM) model to better track interfaces between phases
  - *Explore magnetic field effects on beam and material evolution*
    - Consider wakefield effects on beam propagation and subsequent thermal transport
  - *Continue to improve run coordination*
    - Improve diagnostic outputs and develop composite metrics for simulation guidance and optimizaiton
  - *Consider synchrotron radiation effects on APS-U inline absorbers*
    - Examine downstream synchrotron radiation effects resulting from beam interactions