A Novel Linac Simulation Code AVAS

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Mini-Workshop on Beam Dynamics Simulation for Particle Accelerators

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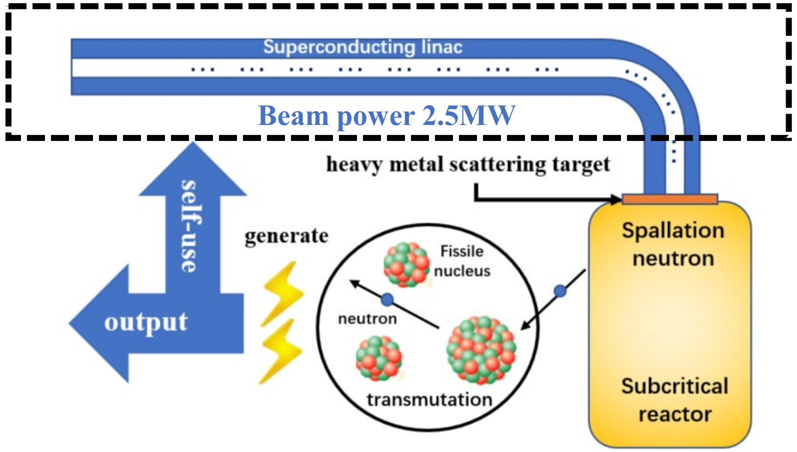
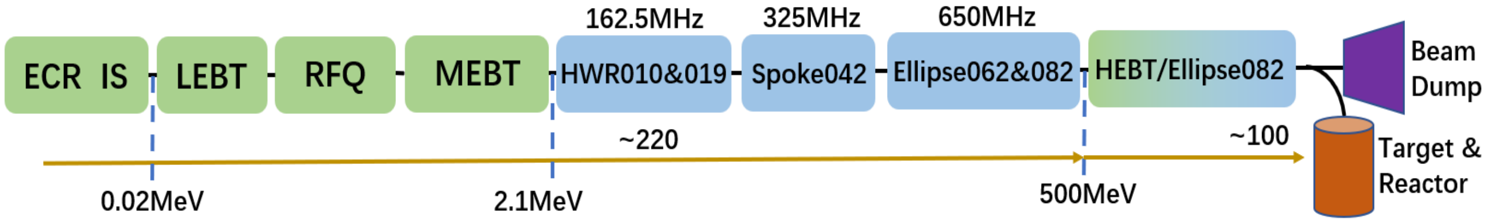
Background and Challenges

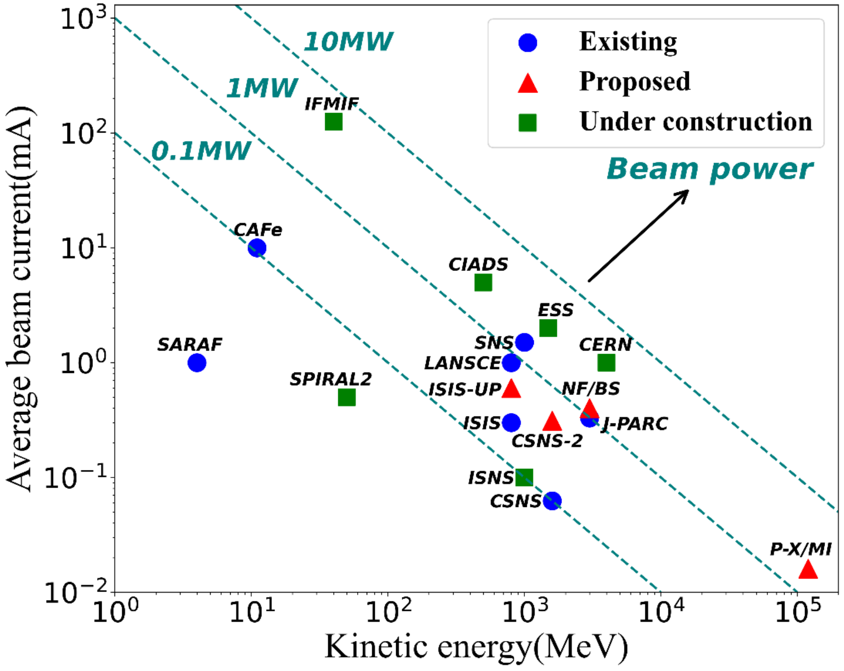
CiADS Schematic



To meet the ever-growing application demands, the energy and beam intensity of accelerators continue to increase.



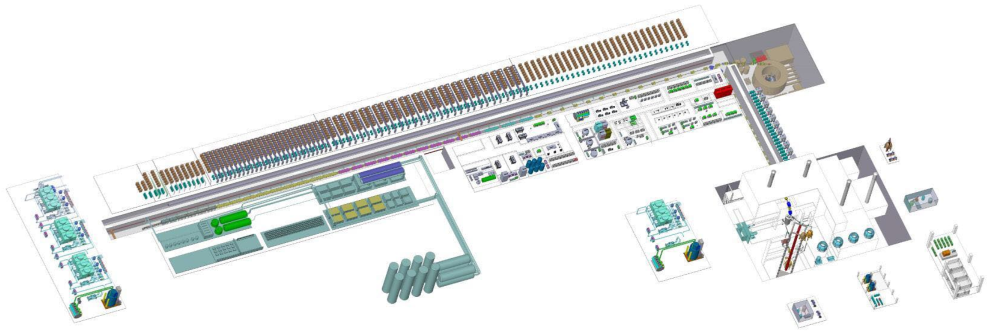
Structure layout of CiADS superconducting linac



Background and Challenges

Commonly Used Beam Simulation Programs

Program	Laboratory	Language	Core Algorithm
TraceWin	CEA Saclay	C++, Python	PIC(PICNIC)
RF-Track	CERN	C++, Octave, Python	Particle to Particle, CIC (Green function method)
PyORBIT	ORNL	C++, Python	PIC(FFT)
IMPACT	LBNL	Fortran90, Python	PIC (Green function method)
Parmila	LANL	Fortran	PIC(SCHEFF)
BEAMPATH	SLAC	Fortran77	PIC(FFT)
TRACK	ANL	-	PIC(FFT)
WARP3D	LLNL	Fortran	PIC(FFT)



Challenges for Accelerator Simulation

1.Computational Complexity: High-intensity ion accelerators exhibit strong nonlinear space charge effects, requiring minutes to hours per simulation.

2.Simulation-Reality Mismatch: Discrepancy between numerical simulations and actual accelerators, making it difficult to closely integrate numerical simulations with accelerator operations.

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Space Charge Effect

Modified PICNIC algorithm: S-PICNIC

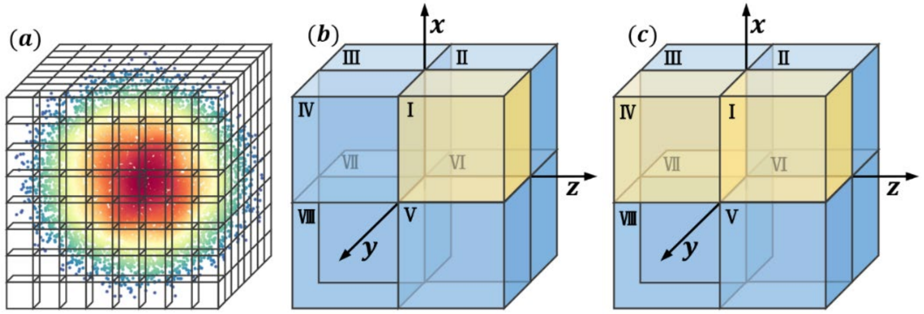
1. **Fully utilize the symmetry of bunch**

   The solution of space charge field is divided into two parts:

   - the solution of symmetric space charge field
   - the correction of asymmetric field component

2. **Neglecting operations that contribute less to the space charge field**

   - Setting thresholds: $TH = RTH \times$ Central node charge
   - Ignoring the contribution of charges below the threshold to the space charge field



The higher the bunch symmetry, the faster the solving speed.

Evaluation Metrics

- To quantify the precision loss from ignoring low-charge grid points

$$\mathrm{MRE} = (\mathrm{MRE_p} + \mathrm{MRE_v})/2$$ **Quantify the difference between two bunch**

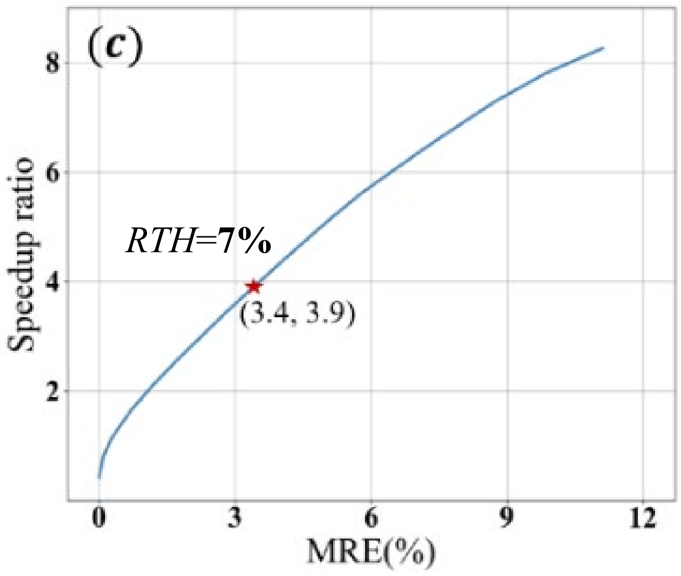
$$\mathrm{MAE_p} = \frac{1}{3}\left(\frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(x_i - x_{0i})^2}}{xSize} + \frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(y_i - y_{0i})^2}}{ySize} + \frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(z_i - z_{0i})^2}}{zSize} \right)$$

$$\mathrm{MAE_v} = \frac{1}{3}\left(\frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(v_{xi} - v_{x0i})^2}}{v_x Size} + \frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(v_{yi} - v_{y0i})^2}}{v_y Size} + \frac{\sqrt{\frac{1}{N_P}\sum_{i=1}^{N_p}(v_{zi} - v_{z0i})^2}}{v_z Size} \right)$$

Space Charge Effect

Test result

- Change *RTH* from 0.05%to20%, observation of the relation between speed and error



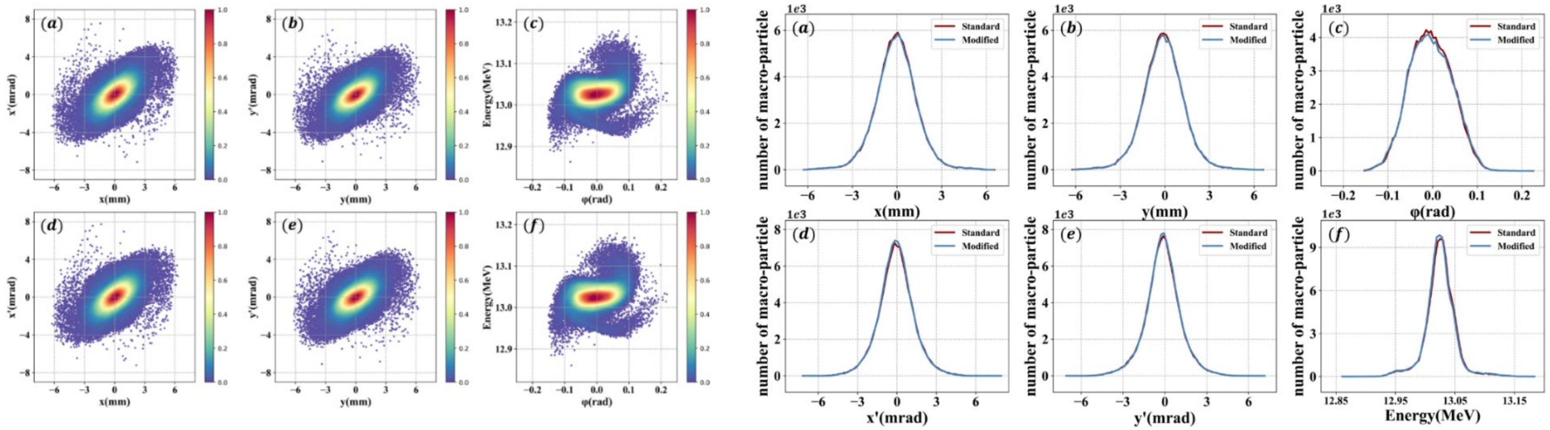
$$\text{Speed up ratio} = \frac{T_1}{T_2}$$

T_1 and T_2 are the time taken by the standard algorithm and the modified algorithm to solve the SC field, respectively

simulation conditions

Macro-particle number: 99940
Intensity: 5mA
Frequency: 162.5MHz
Initial energy: 1.52MeV
length: 13.07m
Grid: $22 \times 22 \times 22$
$\Delta t = 1/(frequency * 100)$
$\boldsymbol{RMS_x = 1.48mm}$
$\boldsymbol{RMS_y = 0.66mm}$

	$Emit_x$	$Emit_y$	$Emit_z$	Energy
PICNIC	0.2281	0.2153	0.0336	13.0278
S-PICNIC	0.2315	0.2179	0.0337	13.0271



Comparison of simulation results between two algorithms when MRE = **3.4%**

Particle Motion

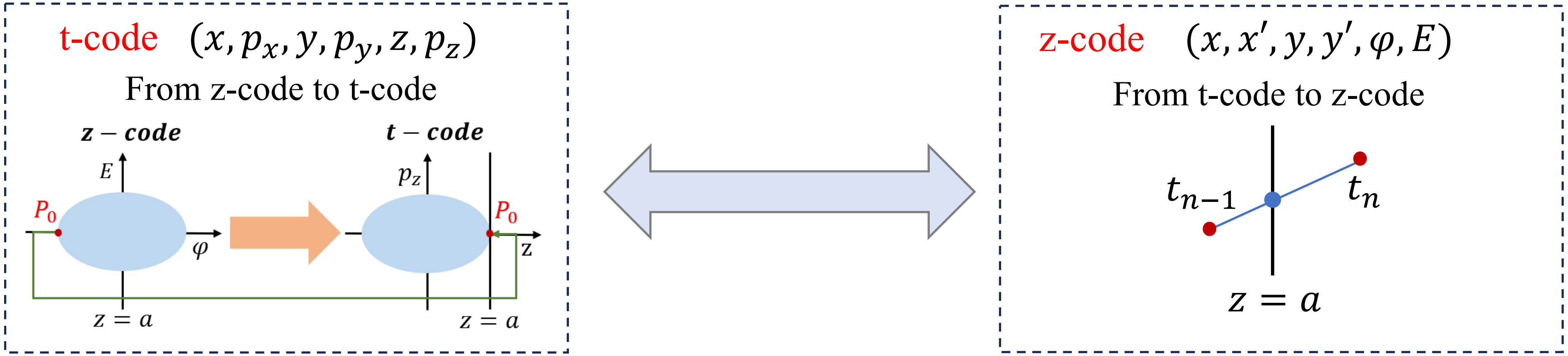
T-code and Z-code

- T-code with time as independent variable ($t \rightarrow t + \Delta t$), and the program saves the distribution of bunch at time t
- Z-code with position as independent variable ($z \rightarrow z + \Delta z$), and the program saves the distribution of bunch on the z=a plane.

Using conditions

- Z-code is used in hard-edged components to use the transfer matrix.
- T-code is used in field map components for more accurate space charge effects calculation.

1. High-precision conversion between z-code and t-code



Key: Ensure that the parameters of the particle passing through the z=a plane are consistent with those before the Conversion.

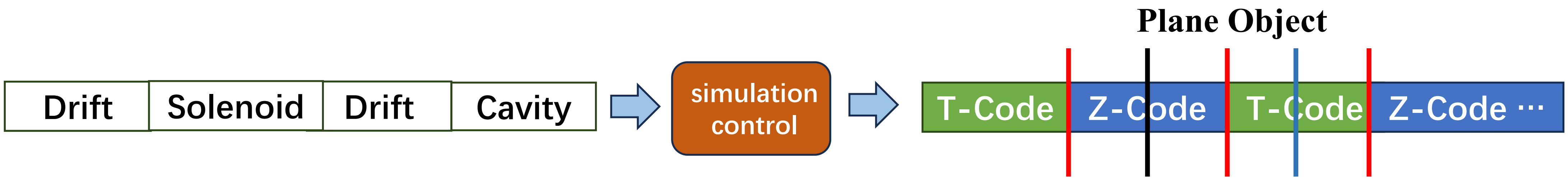
Key: by backing up the bunch information from the previous moment, interpolate to obtain the particle parameters at the z = a plane

Particle Motion

2.Code design that adapts to switching between two modes

Define plane object

- **Functions such as bunch output, mode conversion, and thin lens elements are integrated into plane object.**
- **The bunch will stop at a plane when it encounters a plane object, and will continue to transfer from the plane after executing the operation**



simulation control

- Before the simulation begins, the beamline is divided into T-code segments and Z-code segments according to the element type.
- Insert plane object based on user needs (Output, Mode conversion) and the location of special components (Thin lens).

Unify the implementation of functions and elements across different modes.

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High Performance Computing

AVASX: An ultra-high-speed GPU-based version using CUDA.

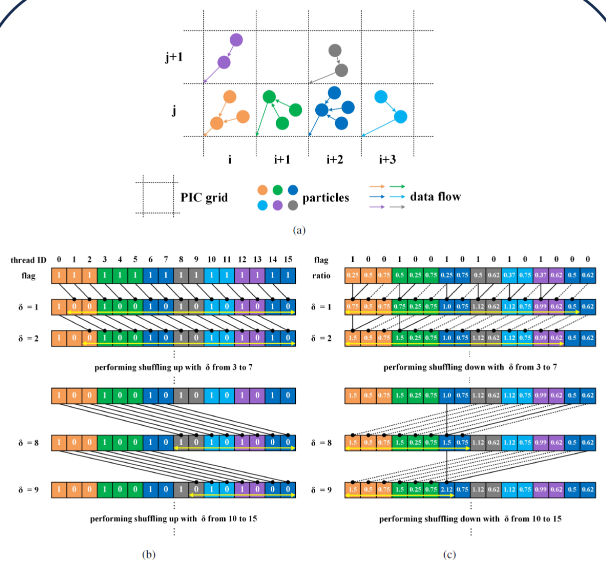
Computational bottleneck

Particle-in-cell (PIC) methods require **numerous particles** to accurately capture the underlying physics.

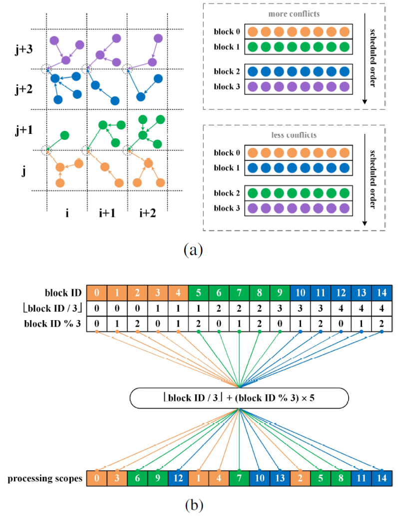
Solution

GPU-Accelerated High-Performance Beam Dynamics Simulation

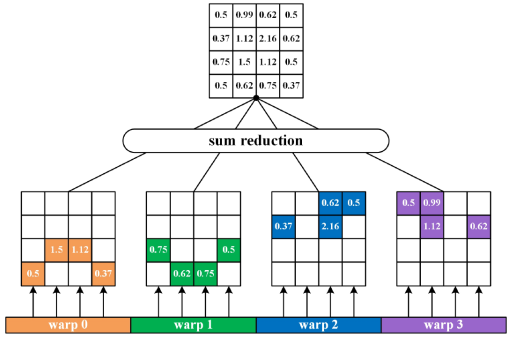
Key Challenges： Memory Access Conflicts in Atomic Operations on GPU Global Memory



Thread Aggregation



Data Processing Range Dispersion



Memory Instance Replication

High Performance Computing

Performance Evaluation

Memory workload metrics, compute and memory throughputs, execution durations, and performance improvements of different kernels in charge deposition calculation.

Employed kernel	Threads to L1 cache			L1 cache to L2 cache		Excessive sector rate (%)	Compute throughput (%)	Memory throughput (GB/s)	Duration (us)	Performance improvement (%)
	Memory requests	Requested sectors	Hit rate (%)	Memory requests	Requested sectors					
kernel-3	250,000	7,832,161	0%	7,691,097	7,832,161	9.9	6.92	51.96	463.01	-
kernel-4	250,016	7,814,976	0%	7,673,911	7,814,976	9.9	14.31	51.96	463.74	-0.16
kernel-5	251,904	7,822,528	0%	7,681,463	7,822,528	9.9	14.37	52.07	463.49	-0.1
kernel-6	250,000	7,832,737	0%	7,692,102	7,832,737	9.9	7.55	56.82	426.5	8.56
kernel-7	250,000	7,869,016	0%	7,842,952	7,869,016	not provided	5.87	19.48	1230	-62.36
kernel-8	250,016	997,324	0%	992,204	997,324	0.01	29.95	167.78	143.55	222.54
kernel-9	251,904	1,004,876	0%	999,756	1,004,876	0.01	56.05	307.71	78.4	490.57
kernel-10	250,016	997,324	0%	992,204	997,324	0.01	45.79	250.32	96.67	378.96
kernel-11	251,904	1,004,876	0%	999,756	1,004,876	0.01	64.63	356.47	68.06	580.3

580% Improvement in Charge Deposition Performance

A100 GPU vs. 56 Core CPU

$N_p = 1,000,000$	CAFe	CiADS
AVASX	16.58 s	45.98 s
AVAS	2.17 h	7.04 h
Speedup	472	550

CAFe

Length: 16.27m $f = 162.5\text{MHz}$

Intensity : 0.27mA $\Delta t = \frac{1}{100 * f}$

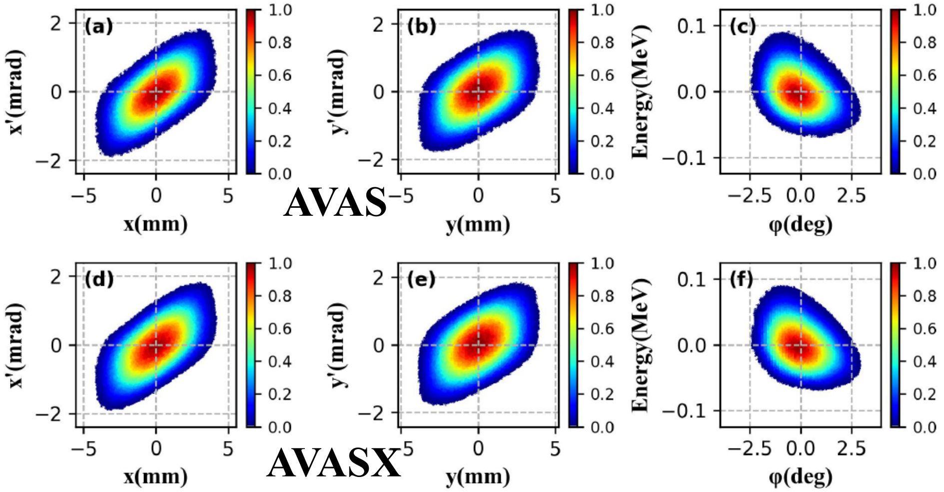
CiADS

Length: 202.75m $f = 162.5\text{MHz}$

Intensity : 5mA $\Delta t = \frac{1}{100 * f}$

Verification

Phase space distributions of the bunch at the exit of the CAFe superconducting section



Bunch parameters at the exit of the CAFe superconducting section, simulated by AVASX and AVAS.

Code	Particle number	Emittance $(\pi \cdot mm \cdot mrad)$			Bunch size (mm)			Energy (MeV)
		$emit_x$	$emit_y$	$emit_z$	$size_x$	$size_y$	$size_z$	
AVASX	1,000,000	0.148	0.152	0.134	1.585	1.486	0.914	16.95
	10,000,000	0.149	0.152	0.134	1.585	1.486	0.914	16.95
AVAS	1,000,000	0.148	0.152	0.134	1.584	1.485	0.914	16.95
	10,000,000	0.149	0.152	0.134	1.584	1.486	0.914	16.95

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Machine Learning Techniques

Physics-Guided Deep Learning Architecture for Beam Phase Space Super-Resolution

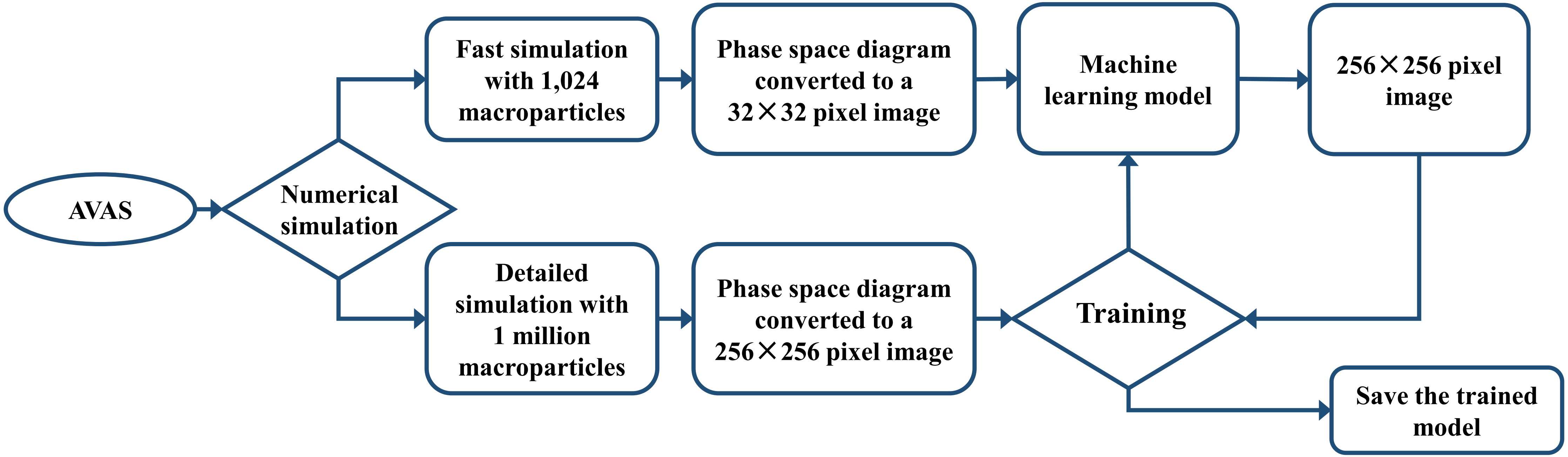
Key Challenge

Incorporating Physical Constraints into Machine Learning to Enhance Model Generalization and Interpretability

Method

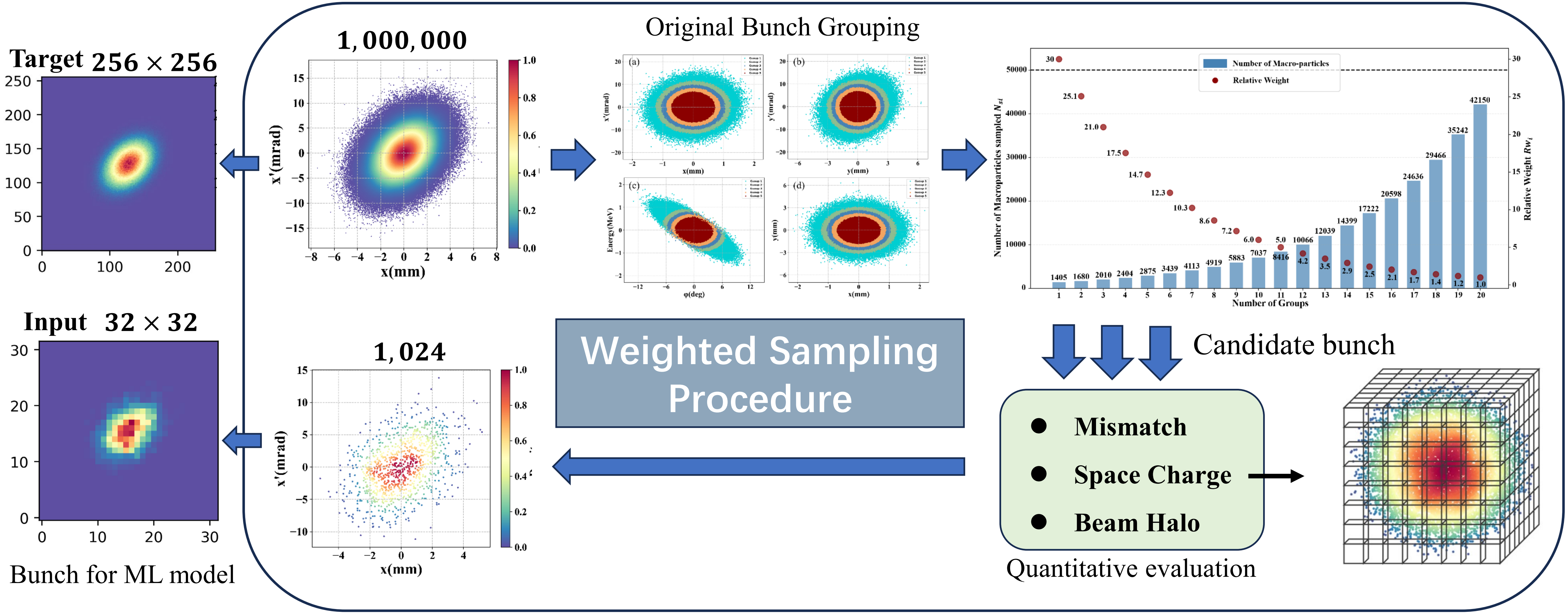
Coarse-grained simulation results obtained through rapid numerical simulations are employed to guide machine learning networks in generating refined results consistent with large-scale multi-particle simulations.

Numerical Simulation Guidance + Machine Learning Model



Physics-Guided Deep Learning Architecture for Beam Phase Space Super-Resolution

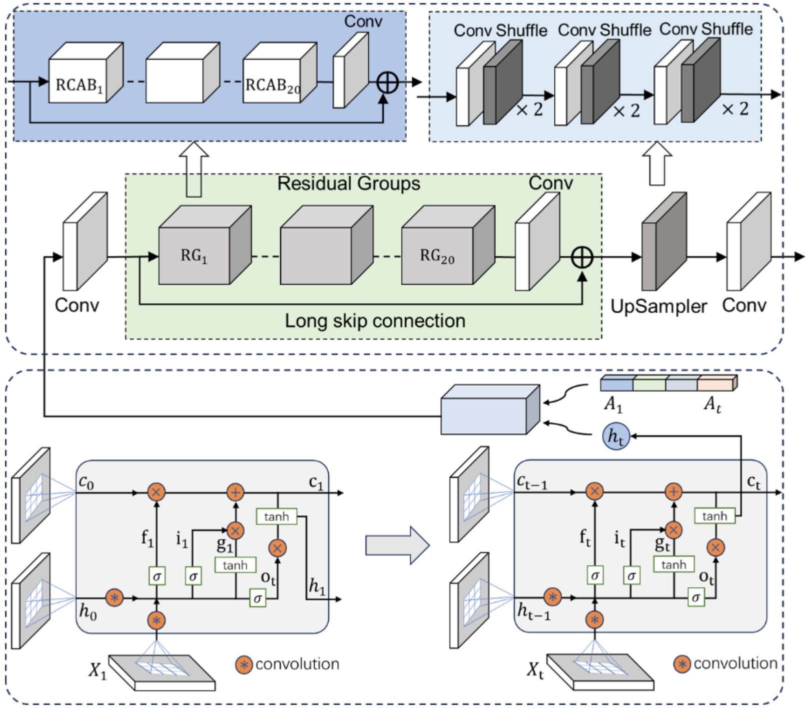
- **Numerical Simulation Guidance**



Machine Learning Techniques

Physics-Guided Deep Learning Architecture for Beam Phase Space Super-Resolution

- **Machine Learning Model**



- **Sample size**

Training set	Independent test set
800 × 200	200 × 200

800 simulation runs, each outputting 200 bunch distributions along the beamline

- **Data set**

CAFe Superconducting Section

Macro-particle number: 1,000,000
1024

Intensity: 5mA
Frequency: 162.5MHz
Length: 13 m

Error boundaries of elements

Element Type	Cavity	Solenoid
Rotation Error	$\mp 4mrad$	$\mp 2mrad$
Translation Error	$\mp 1.0mm$	$\mp 0.5mm$
Field amplitude Error	$\mp 1\%$	$\mp 4\%$
Phase Error	$\mp 1deg$	

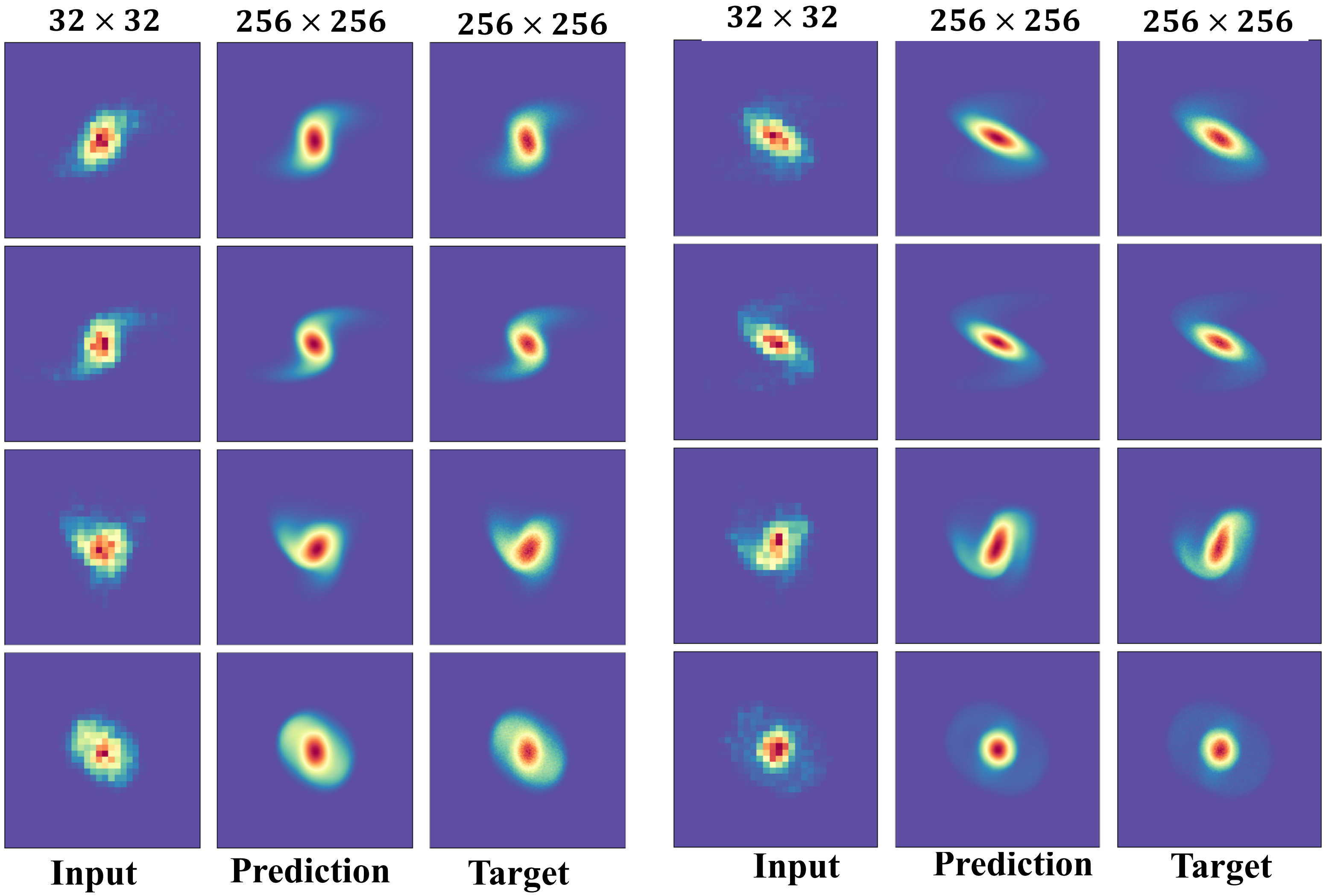
Initial bunch error

Current Error	Beam mismatch	Emittance growth
$\mp 2.5mA$	50%	50%

Machine Learning Techniques

Physics-Guided Deep Learning Architecture for Beam Phase Space Super-Resolution

Numerical results | **Generalization (Doubled error)**



R^2=0.991

SSIM=0.987

SSIM: Structural Similarity Index

Summary

1.The number of particles was reduced from 1,000,000 to 1,024.

2.Next, real beam diagnostic data will be incorporated to reconstruct actual beam information.

R^2 =0.981

SSIM=0.984

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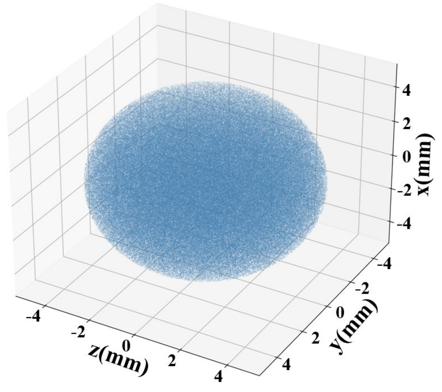
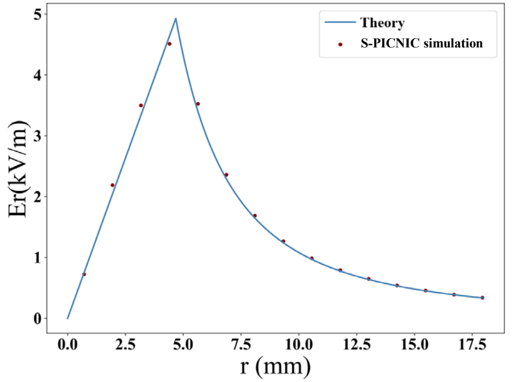
Verification

Analytical Solution Test

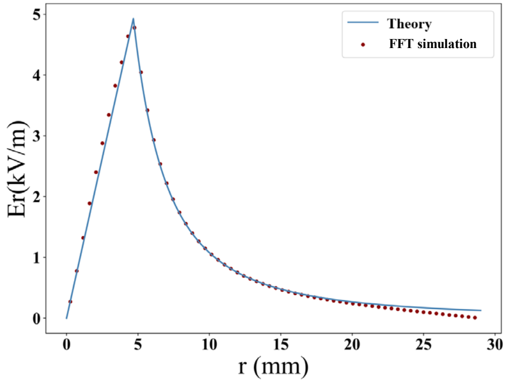
Radial Field Distribution of a Uniform Spherical Bunch



$$E_1 = \rho r / 3\varepsilon_0 \qquad r < R$$
$$E_2 = R^3 \rho / 3\varepsilon_0 r^2 \qquad r > R$$



Nodes: $30 \times 30 \times 30$
Mesh size: $[-5R_{RMS}, 5R_{RMS}]$

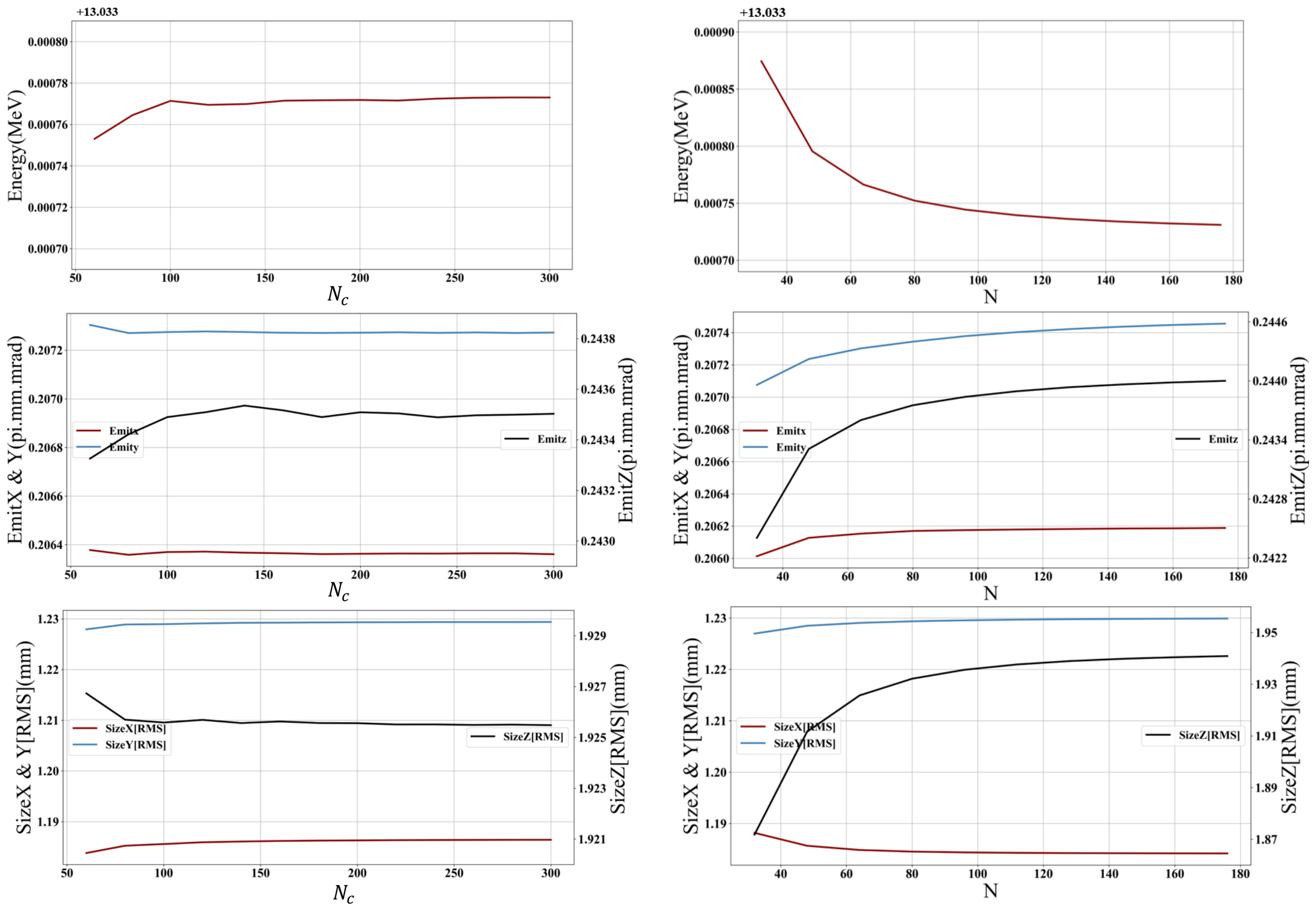


Nodes: $128 \times 128 \times 128$
Mesh size: $[-8R_{RMS}, 8R_{RMS}]$

Convergence test

Beam Transport Simulation in the CAFe Superconducting Section

I = 5mA, Freq = 162.5MHz, E = 1.5MeV, Total length 13.07m



Time step $\Delta t = 1/(N_c * f)$ Number of nodes

Verification

Benchmark

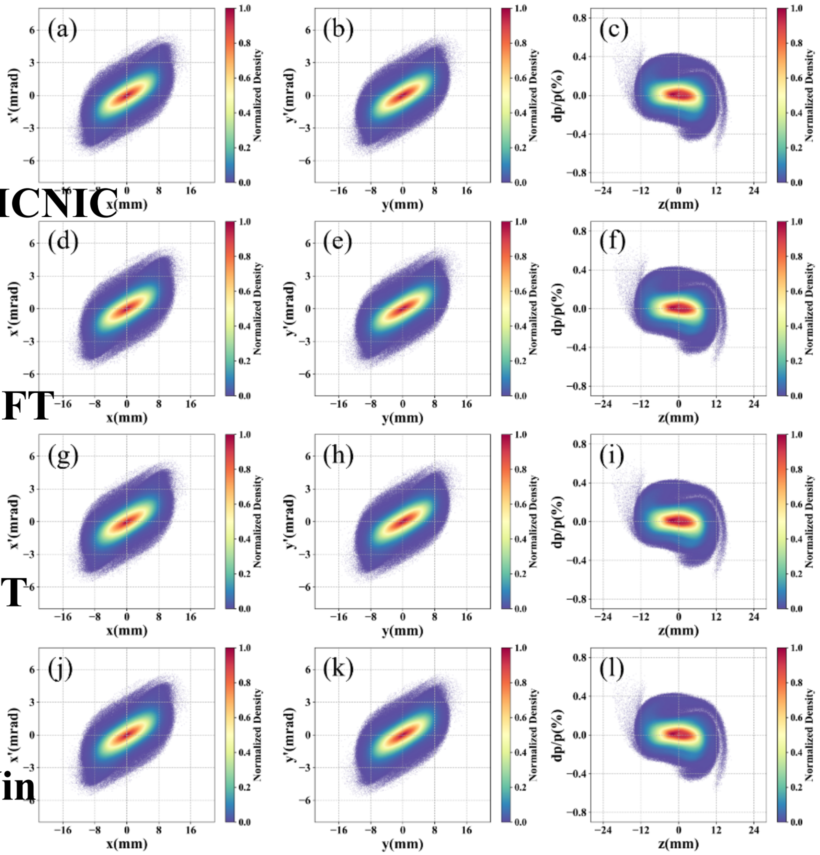
Beam Transport Simulation Through the 100 mA Beamline

AVAS-SPICNIC

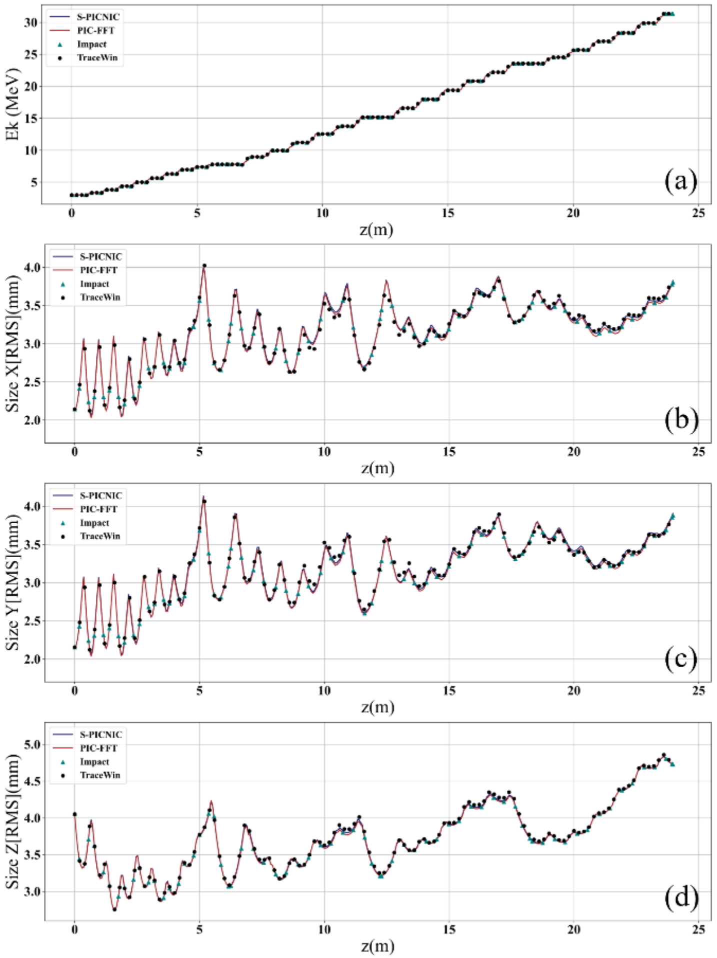
AVAS-FFT

Impact-T

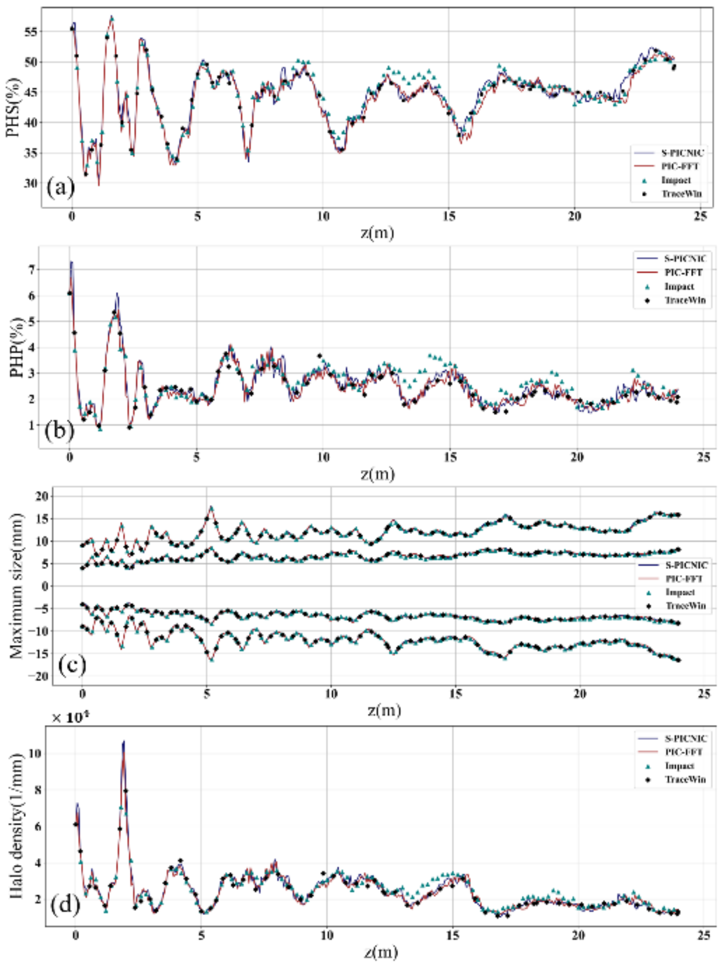
TraceWin



Phase space of exit bunch



Envelope Parameter Deviation < 1.5%

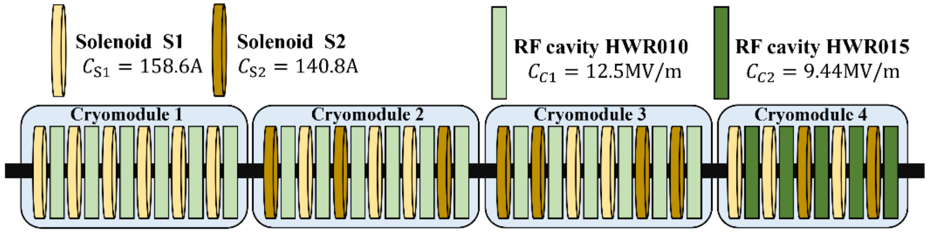


Beam Halo Parameter Deviation < 3.5%

Verification

Experimental Verification

Numerical Simulation

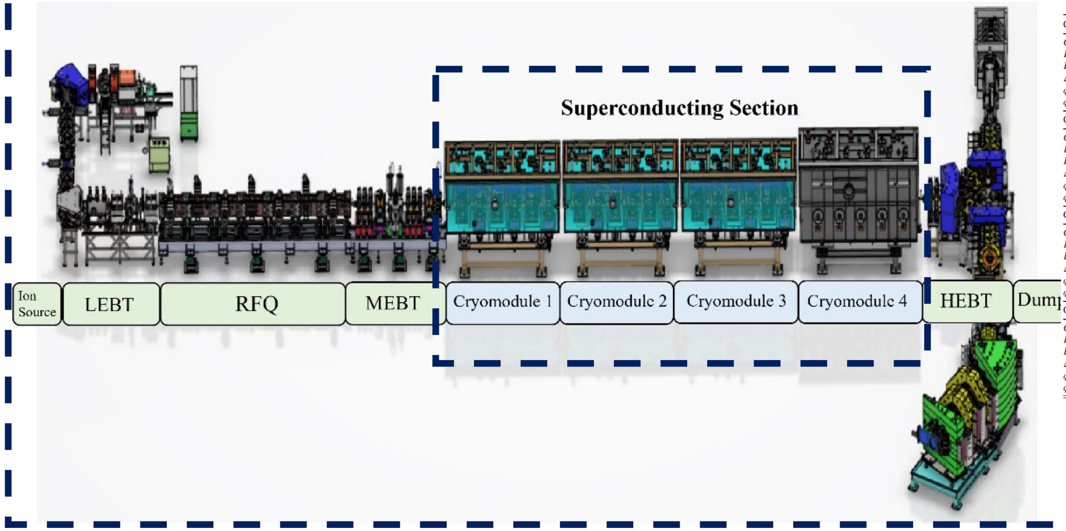


Parameter Calibration

$$\begin{cases} I_{s,i} = C_{s,i} K_i \\ E_{pk,i} = C_{c,i} K_i \end{cases},$$

$$\varphi_{rf} = \varphi_v + \Delta\varphi + n \times 360.$$

Preset Accelerator Operating Parameters



CM1 Cavity						
$C_{c1} = 12.5$	1–1	1–2	1–3	1–4	1–5	1–6
K	1.28	1.2	1.8	1.6	1.5	1.9
E_{pk}	16	15	22.5	20	18.8	23.8
$\Delta\varphi$ (deg)	116	148	44	83	107	–36
φ_v (deg)	–171	–140	100	42	45	93
φ_{rf} (deg)	–55	8	144	124	152	56
CM2 Cavity						
$C_{c1} = 12.5$	2–1	2–2	2–3	2–4	2–5	2–6
K	2	1.86	2	2.2	2.4	2
E_{pk}	25	23.2	25	27.5	30.0	25.0
$\Delta\varphi$ (deg)	–146	–139	103	171	–77	–76
φ_v (deg)	147	7.2	–45	–30	17	137
φ_{rf} (deg)	0.8	–132	59	141	–60	61
CM3 Cavity						
$C_{c1} = 12.5$	3–1	3–2	3–3	3–4	3–5	3–6
K	2.1	2	2.3	2.24	1.76	2
E_{pk}	26.2	25	28.7	28	22.0	25.0
$\Delta\varphi$ (deg)	–143	–117	–50	–96	–15	41
φ_v (deg)	–174	98	46	46	86	107
φ_{rf} (deg)	42	–19	–4	–50	71	148
CM4 Cavity						
$C_{c2} = 9.44$	4–1	4–2	4–3	4–4	4–5	...
K	2.9	1.22	0	0	0	...
E_{pk}	27.4	11.5	0	0	0	...
$\Delta\varphi$ (deg)	145	149	–37	–74	...	...
φ_v (deg)	111	10	...	...	...	...
φ_{rf} (deg)	–104	159	...	...	...	...

CM1 Solenoid						
$C_{s1} = 158.6$	S1	S1	S1	S1	S1	S1
K	0.8	0.78	0.81	0.88	0.75	0.98
$I_s(A)$	126.9	123.7	128.5	139.6	119.0	155.4
CM2 Solenoid						
$C_{s2} = 140.8$	S2	S1	S2	S1	S1	S2
K	0.87	0.95	0.47	1.05	0.9	0.9
$I_s(A)$	122.5	150.7	66.0	166.5	142.7	126.7
CM3 Solenoid						
$C_{s1} = 158.6$	S2	S2	S1	S1	S2	S2
K	0.9	0.84	0.87	0.95	0.82	0.92
$I_s(A)$	126.7	118.3	138.0	150.7	115.5	129.5
CM4 Solenoid						
$C_{s2} = 140.8$	S1	S1	S2	S1	S2	-
K	1.0	0.99	0.98	0.95	0.78	-
$I_s(A)$	159.0	157.0	138.0	150.7	109.8	-

$^{40}Ar^{12+}$

Simulated Energy：
186.6 MeV

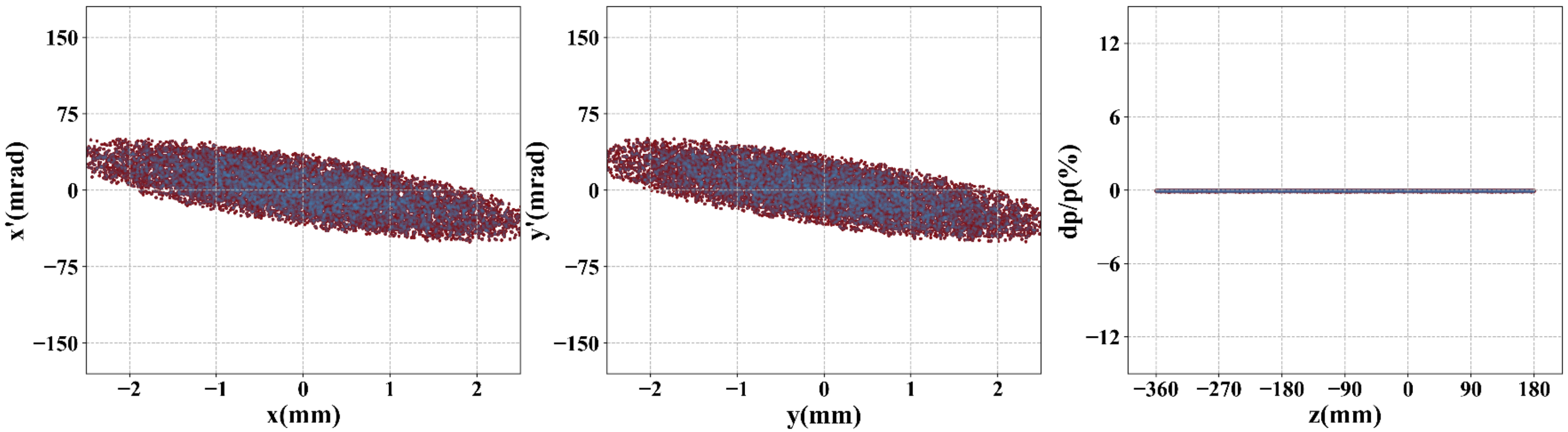
Measured Energy ：
187.5 MeV

Energy Deviation < 0.5%, with No Observable Beam Loss

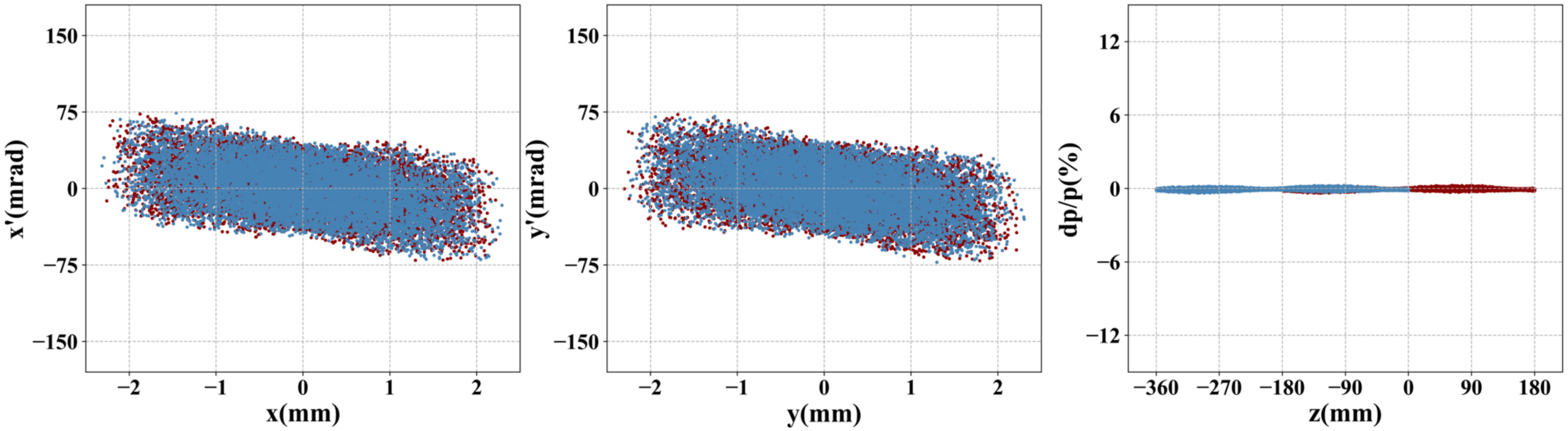
Application

Multi-bunch transmission

Initial Bunch



Simulation of DC beam transport consisting of mixed protons and negative hydrogen ions in an RFQ



Display H^- particles within [-360°, 0°]

Display protons within [-180°, 180°]

Display only particles within one period

Application

Muon Beam Transport

Simulate beam transport with large energy spread and angular divergence

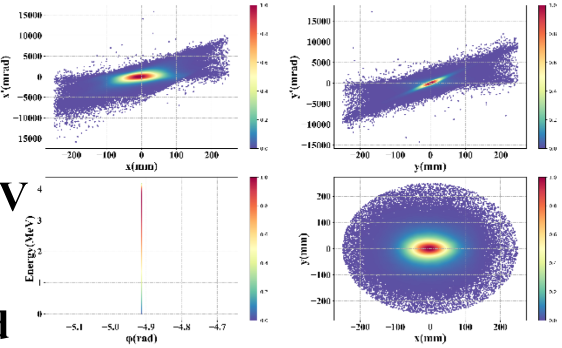
Initial Bunch

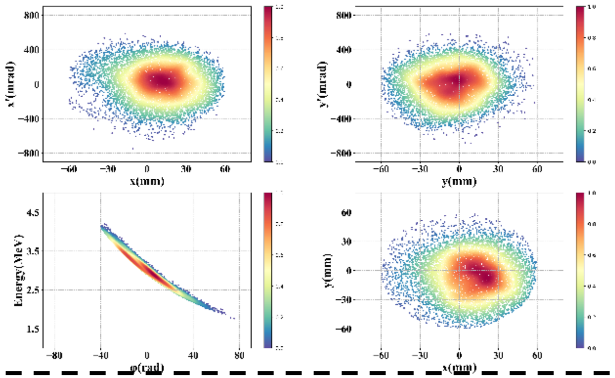
N_p: 480,000

Initial Energy:0 - 4.2MeV

Angular divergence:

<15.8rad





Exit bunch

N_p: 9611

Energy： 1.7-4.2MeV

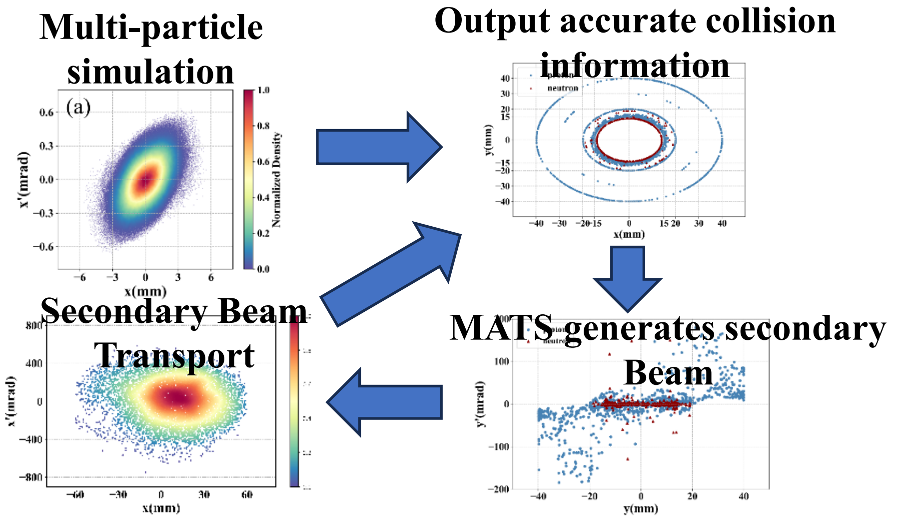
Angular divergence：

<0.58rad

Multi-physics Simulation

AVAS (Multi-particle simulation) → Mats (Secondary Beam generation) ⇄ AVAS (Secondary Beam Transport)

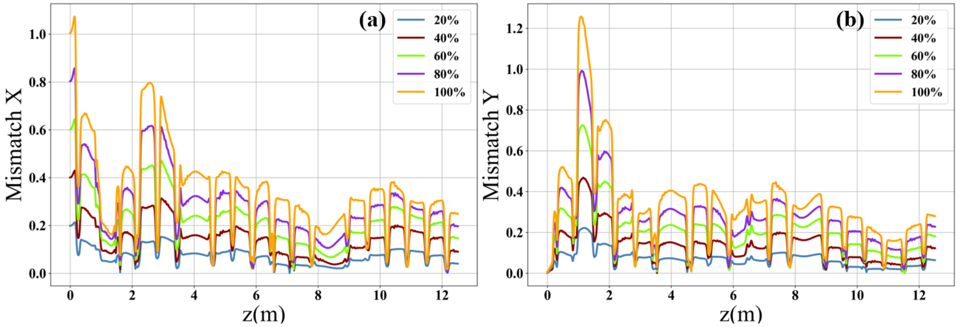
Simulation Workflow



Application

Error study

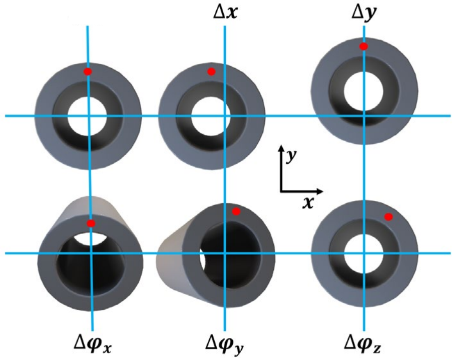
Beam parameter sensitivity analysis

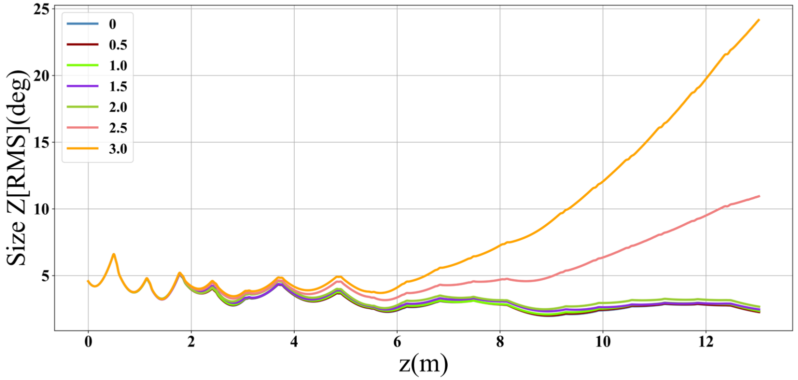


Relationship between entrance bunch mismatch and mismatch along the beamline

Analysis of elements error effects on beam transport

Translation and rotation errors of elements

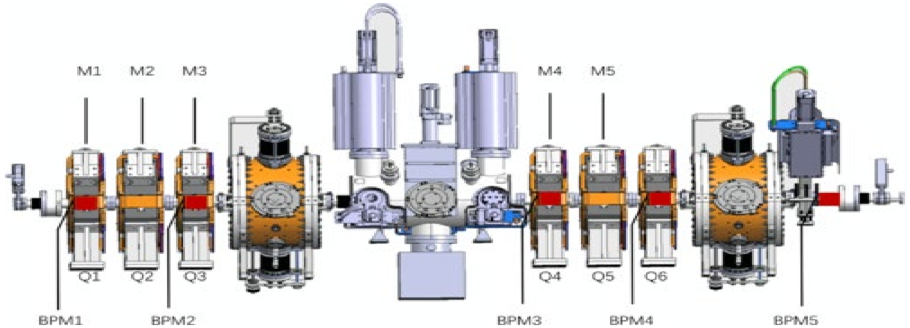




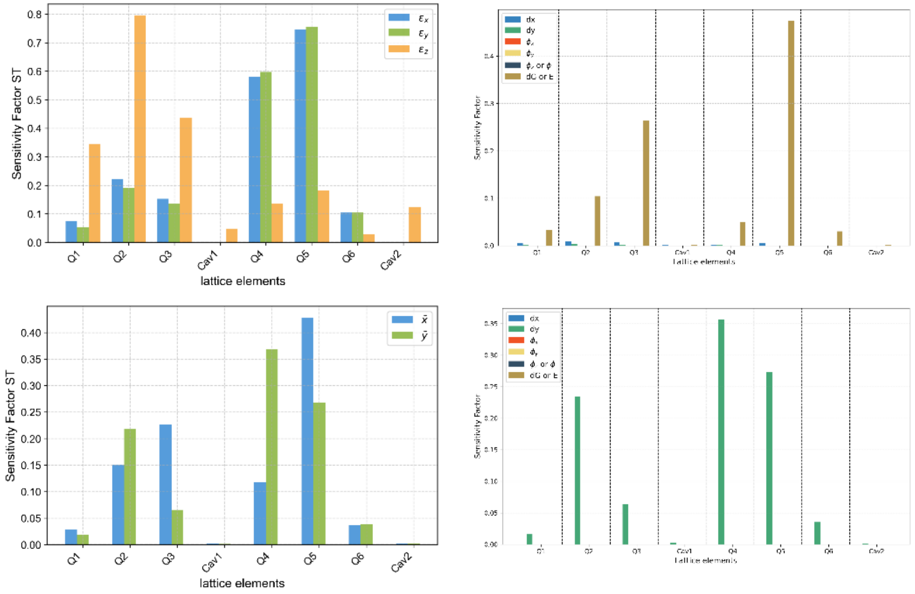
Variation of longitudinal phase width along the beamline with different RF cavity Epk and phase errors

Engineering analysis

Sensitivity-based quantitative analysis of the error-beam quality relationship



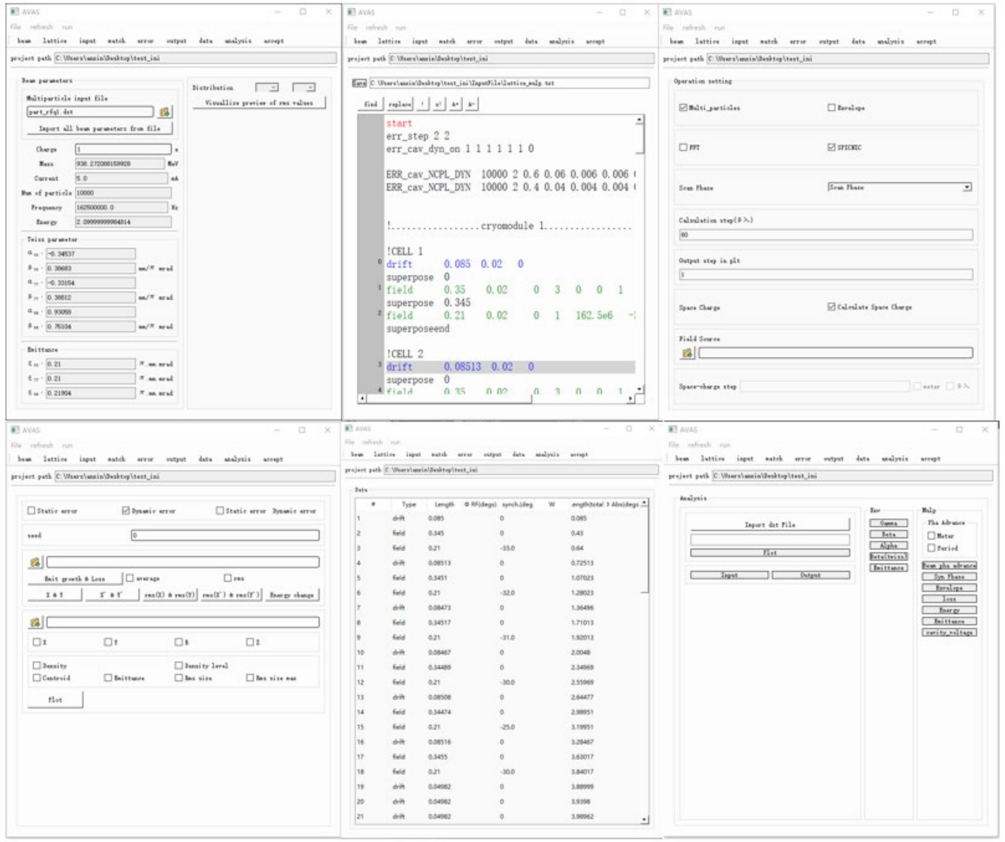
Engineering analysis of the CAFe2 MEBT section



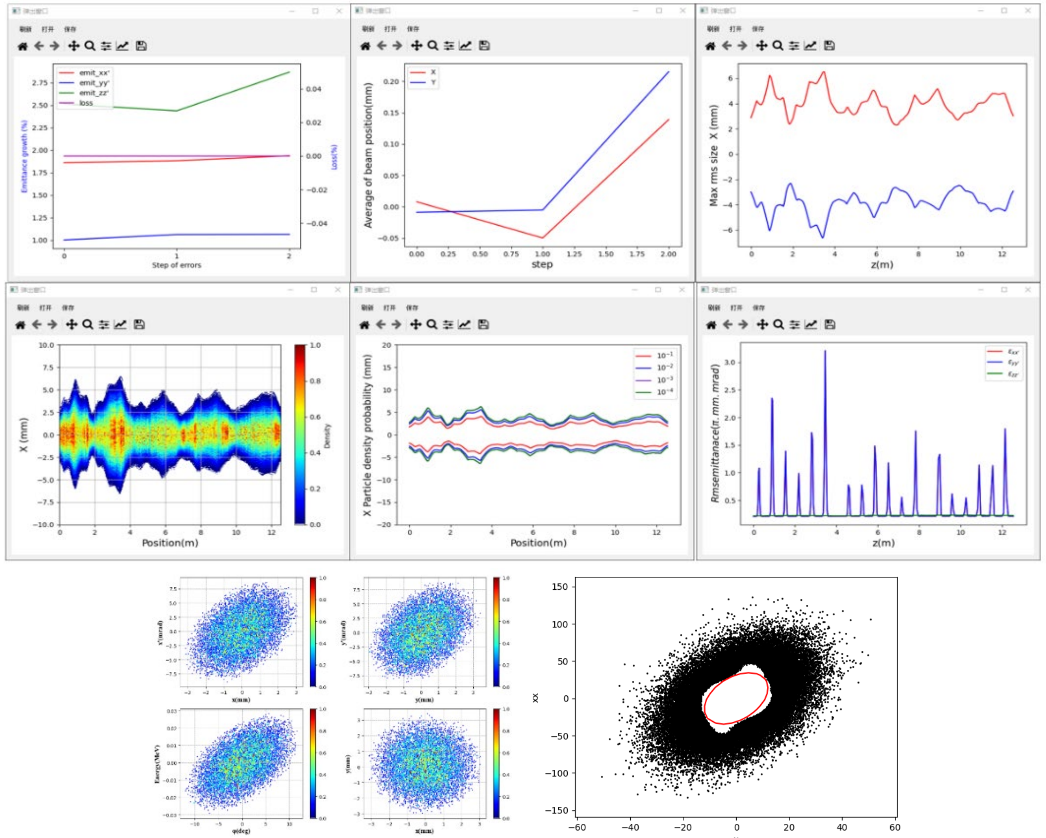
Application

Desktop software

AVAS is a cross-platform software supporting Windows and Linux systems, incorporating a variety of accelerator elements. It features comprehensive capabilities including multi-particle tracking simulation, error analysis, acceptance calculation, transport of particles with large energy spread and angular divergence, and mixed-species beam transport.



Graphical user interface



Data post-processing

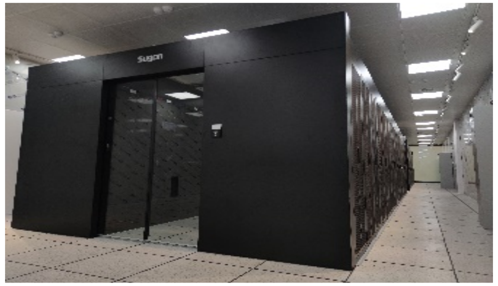
Application

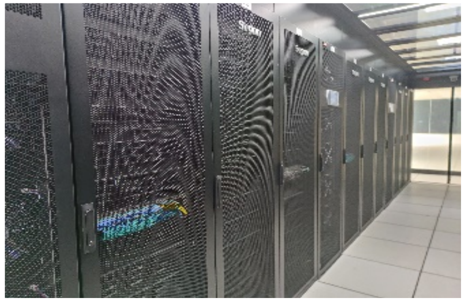
Cloud simulation platform

Computing resources of Dongjiang Laboratory Supercomputing Center

CPU Infrastructure: 14,000+ cores providing peak performance of 1.820 PFLOPS in single precision (FP32) and 0.910 PFLOPS in double precision (FP64);

GPU Infrastructure: 72 NVIDIA A100 40GB SMX4 and 88 A100 40GB PCIe accelerators with aggregate performance exceeding 0.456 PFLOPS (FP32) and 0.228 PFLOPS (FP64).





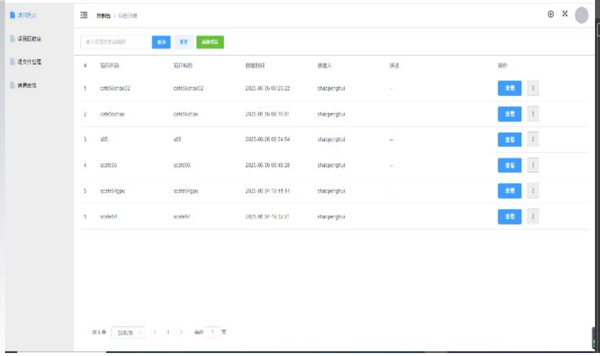
CiADS superconducting segment

N_p: 1,000,000
Length: 202.75m
Beam intensity: 5mA
Frequency: 162.5MHz
Initial energy: 2.1MeV
time step: $\Delta t = 1/(f * 100)$
Output energy: 621.1MeV

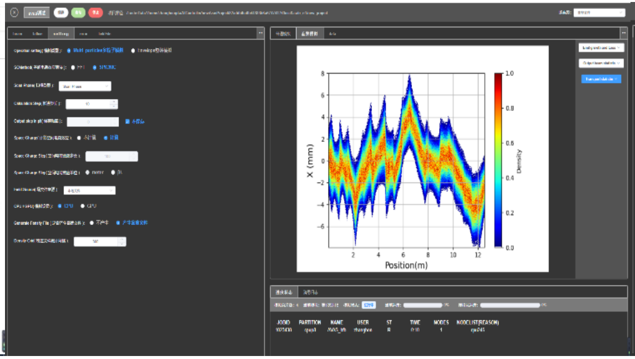
Simulation time

7.04h → 45.98s

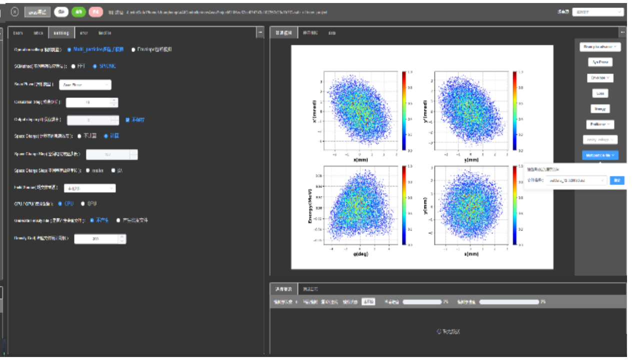
User login



Project management



Parameter Settings



Data post-processing

Summary

群聊：avas用户交流群

该二维码7天内(11月6日前)有效，重新进入将更新

Key Innovations

- **S-PICNIC Algorithm**: 3.9× speedup by exploiting bunch symmetry
- **Hybrid T-code/Z-code**: Seamless switching between tracking modes for optimal accuracy
- **GPU Acceleration (AVASX)**: 470-550× faster than CPU, reducing simulation time from hours to seconds
- **Physics-Guided ML**: Super-resolution model (R^2=0.991) enabling fast multi-particle predictions

Verification & Applications

- Validated against analytical solutions, TraceWin, Impact-T (< 1.5% deviation)
- Experimental verification: < 0.5% energy error, no beam loss
- Applications: Error analysis, multi-bunch transport, mixed-species beams, muon beamlines

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(Physical modeling)

Thanks for your attention

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