Efficient Particle in Cell Simulations of the FRIB Front-End

FRIB

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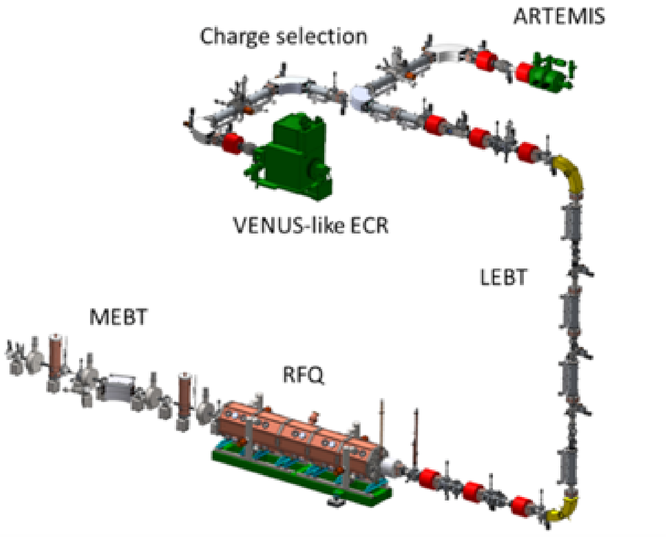
Facility for Rare Isotope Beams (FRIB): front end soon begins early commissioning

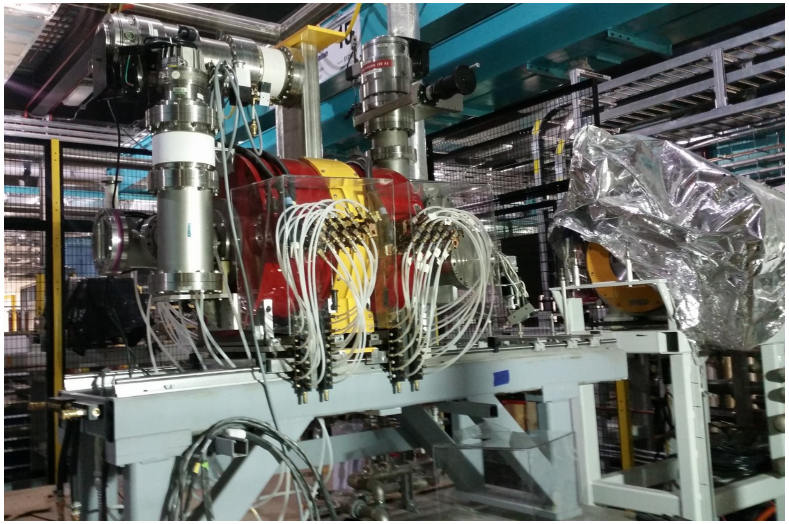
Highlights:

- Sep 2016: Ion source beam commissioning start
- Dec 2016: RFQ high power test start
- Feb 2017: RFQ beam commissioning start
- May 2018: Linac segment 1 beam commissioning start
- 2021: Start of user operation and beam power ramp up

FRIB Front End



Artemis ECR Source now installed, Front end under assembly



Beamline of the FRIB Front End

Ions

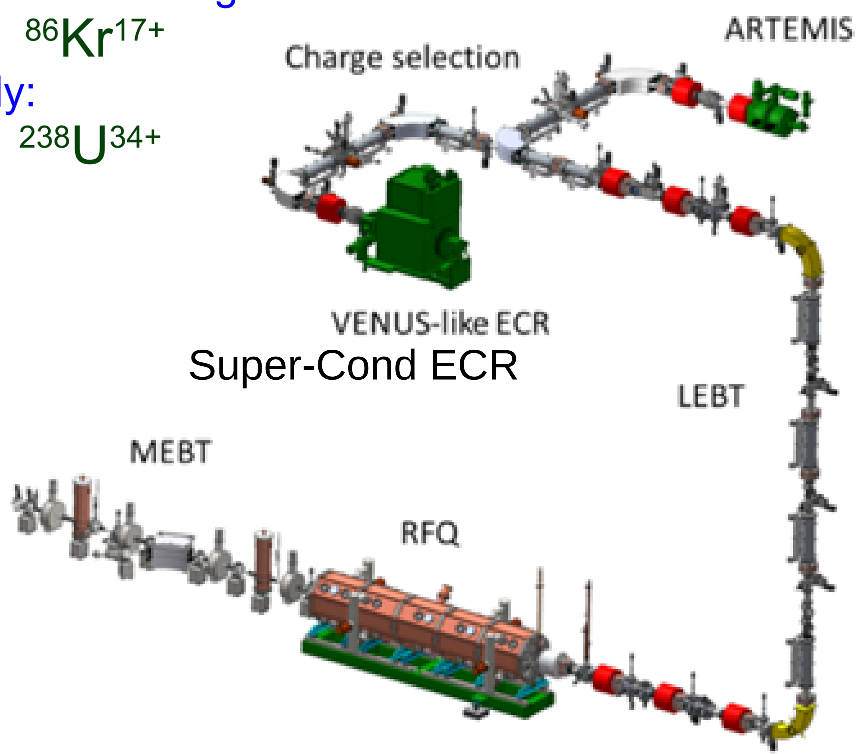
Early Commissioning:

$^{36}Ar^{18+}$ $^{86}Kr^{17+}$

Ultimately:

$^{238}U^{33+}$ $^{238}U^{34+}$

Normal-Cond ECR



Super-Cond ECR

- ECR Ion Source
- Short Solenoid
- ES Accel Gap
- Solenoid
- Magnetic Dipole
- ESQ Triplets
- …
- Ultimately to RFQ

Initial simulations through species selection

Many types of lattice elements to model up to RFQ:

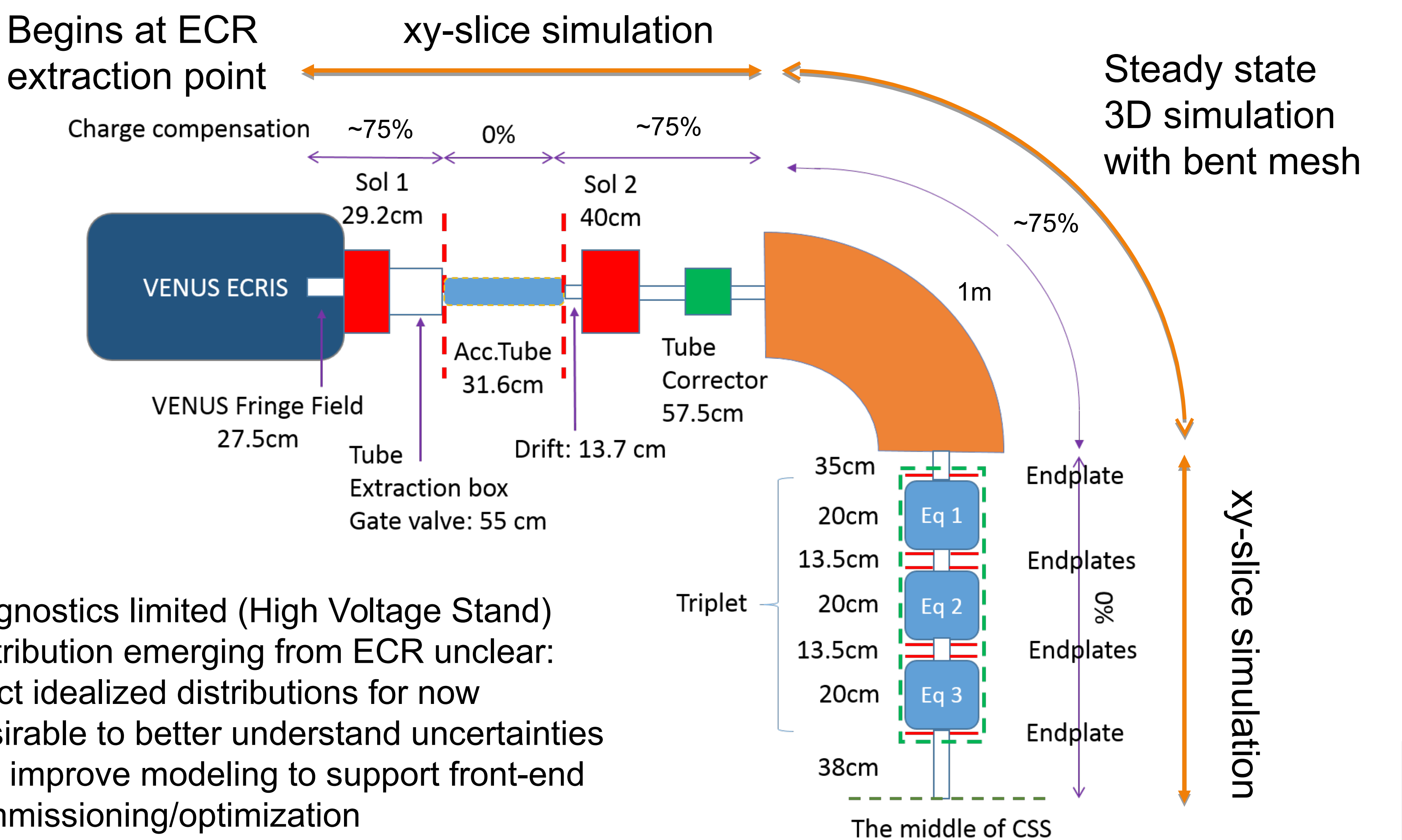
Solenoids	Grated Electrostatic Gap	Collimation Electrodes
Magnetic Dipoles	Electric Dipoles	
Electric Quadrupoles	Bunching Cavities	RFQ

Intense, DC multi-species ion beam emerging from ECR ion sources with part electron neutralization in magnetic optical elements

Overview: Warp PIC Simulations

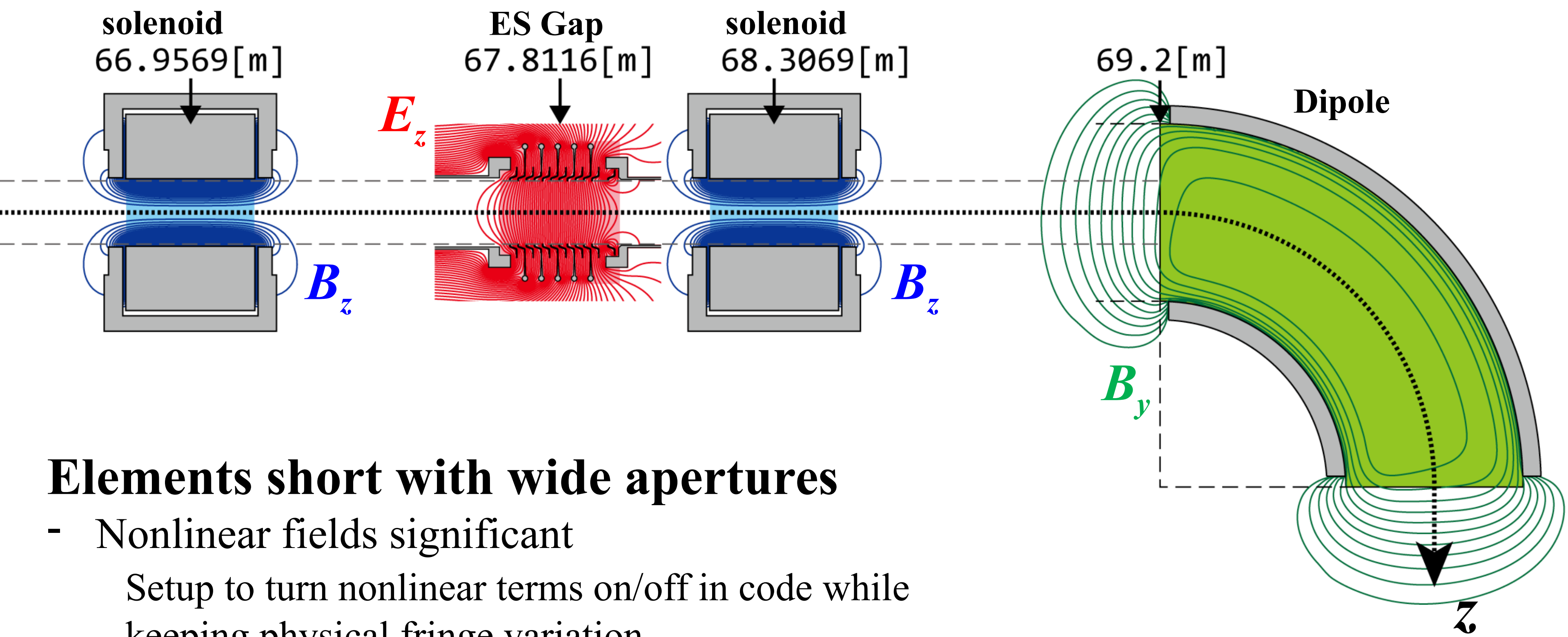
Apply open source Warp PIC code tools for adaptable/efficient simulation on front end

- Formulation for many species with part electron neutralization
- xy transverse slice with 3D element fields
- Full 3D steady state in linked simulations where potential 3D self-field issues



- Diagnostics limited (High Voltage Stand)
- Distribution emerging from ECR unclear: inject idealized distributions for now
- Desirable to better understand uncertainties and improve modeling to support front-end commissioning/optimization

Lattice elements modeled at high levels of detail for importing into simulations



Elements short with wide apertures

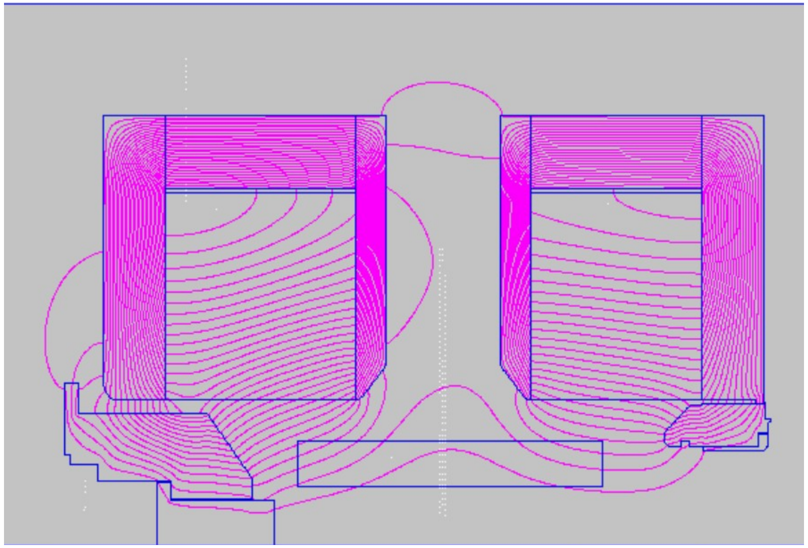
- Nonlinear fields significant
  - Setup to turn nonlinear terms on/off in code while keeping physical fringe variation
- Fringe fields neighboring elements can overlap
  - Modeled in code: find implications

Formulated to apply filed data from numerous optics design codes

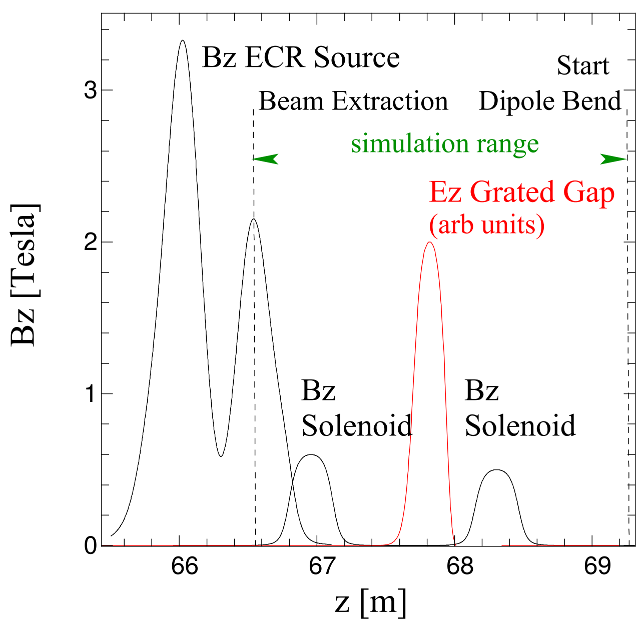
CST Studio   Opera   Maxwell   Poisson

Example details of lattice element models: ECR source

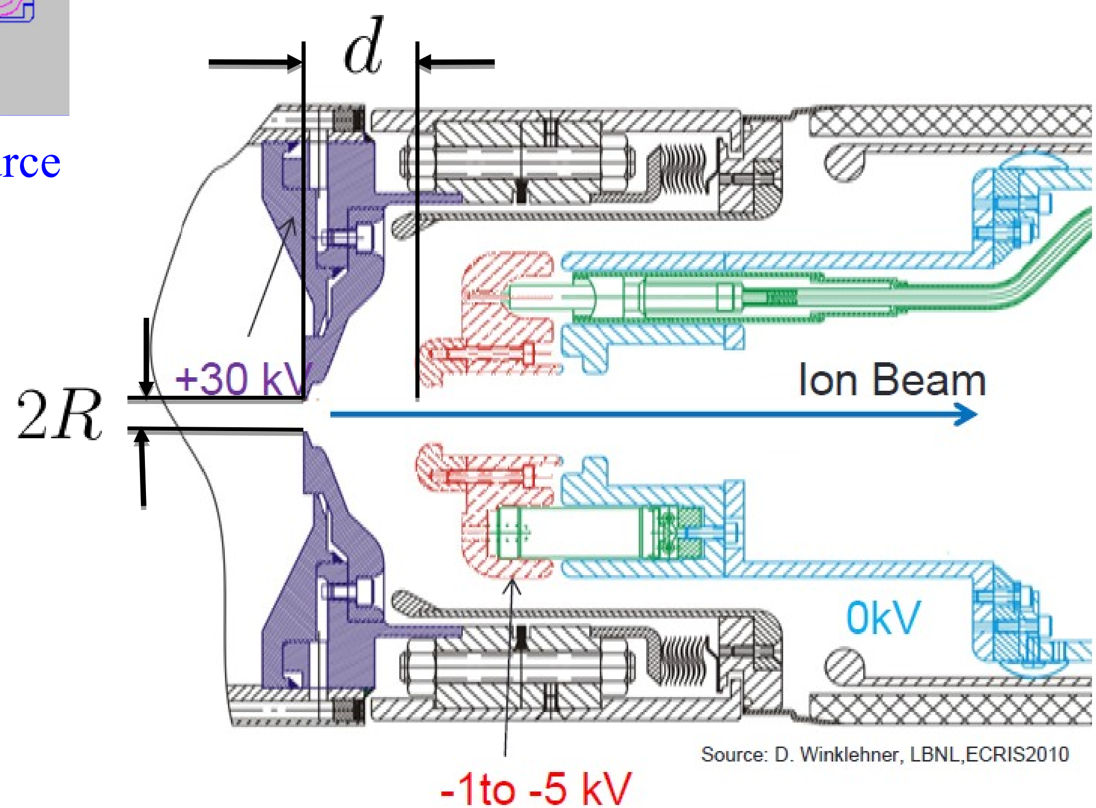
Poisson Model: Solenoid of NC Artemis ECR



Axial Field Overlaps Near ECR Source



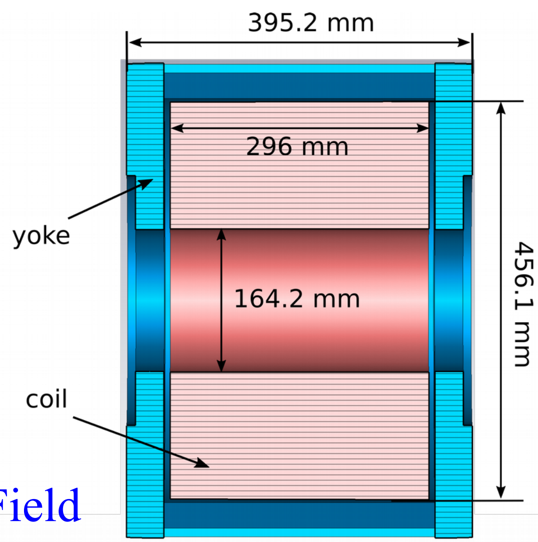
Puller Electrodes of SC Venus ECR



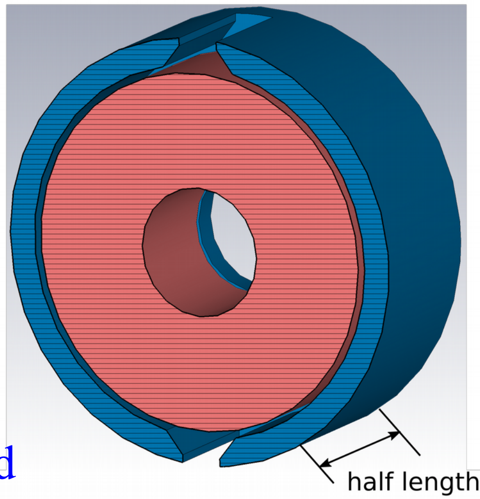
Source: D. Winklehner, LBNL,ECRIS2010

Example details of lattice element models: Solenoids

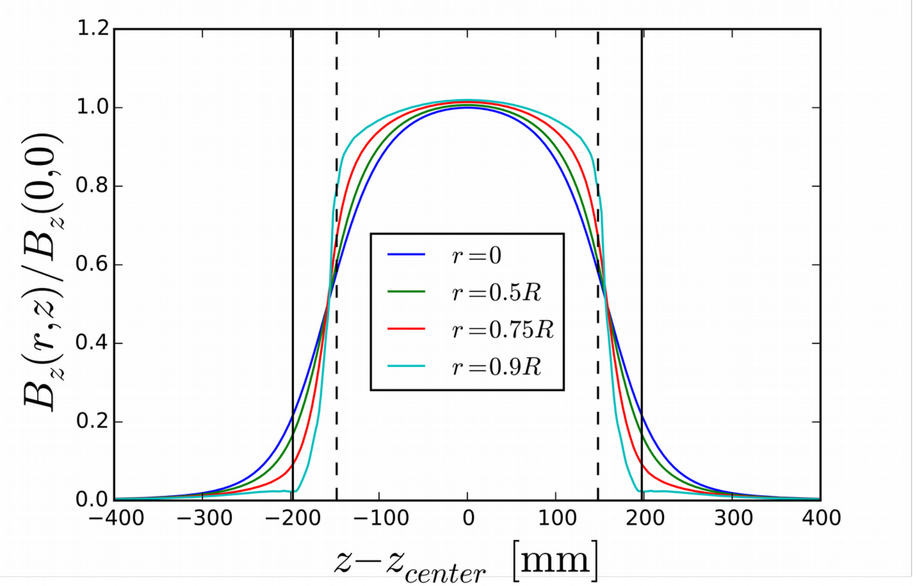
Cross Section



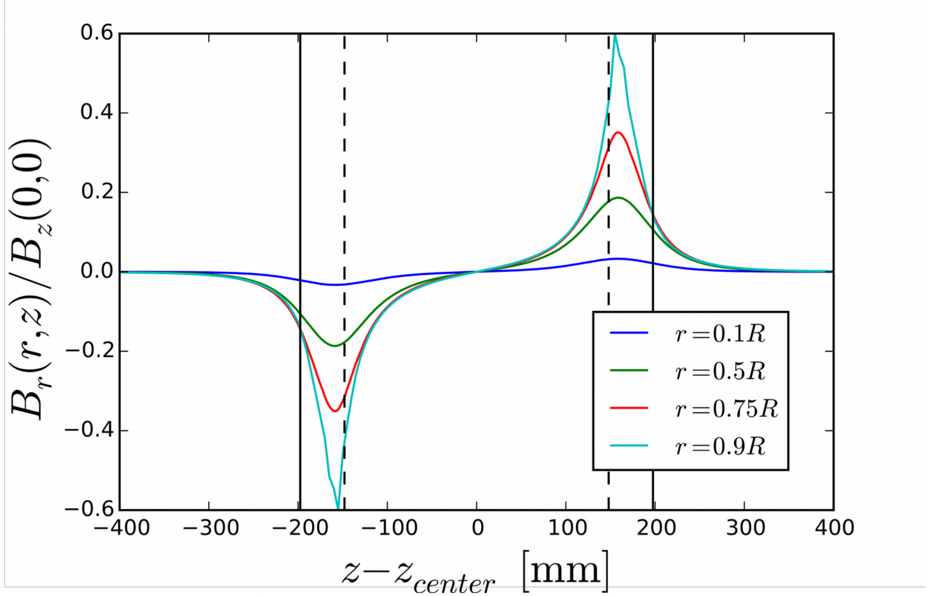
Half (Cut) Perspective View



Axial Field



Radial Field

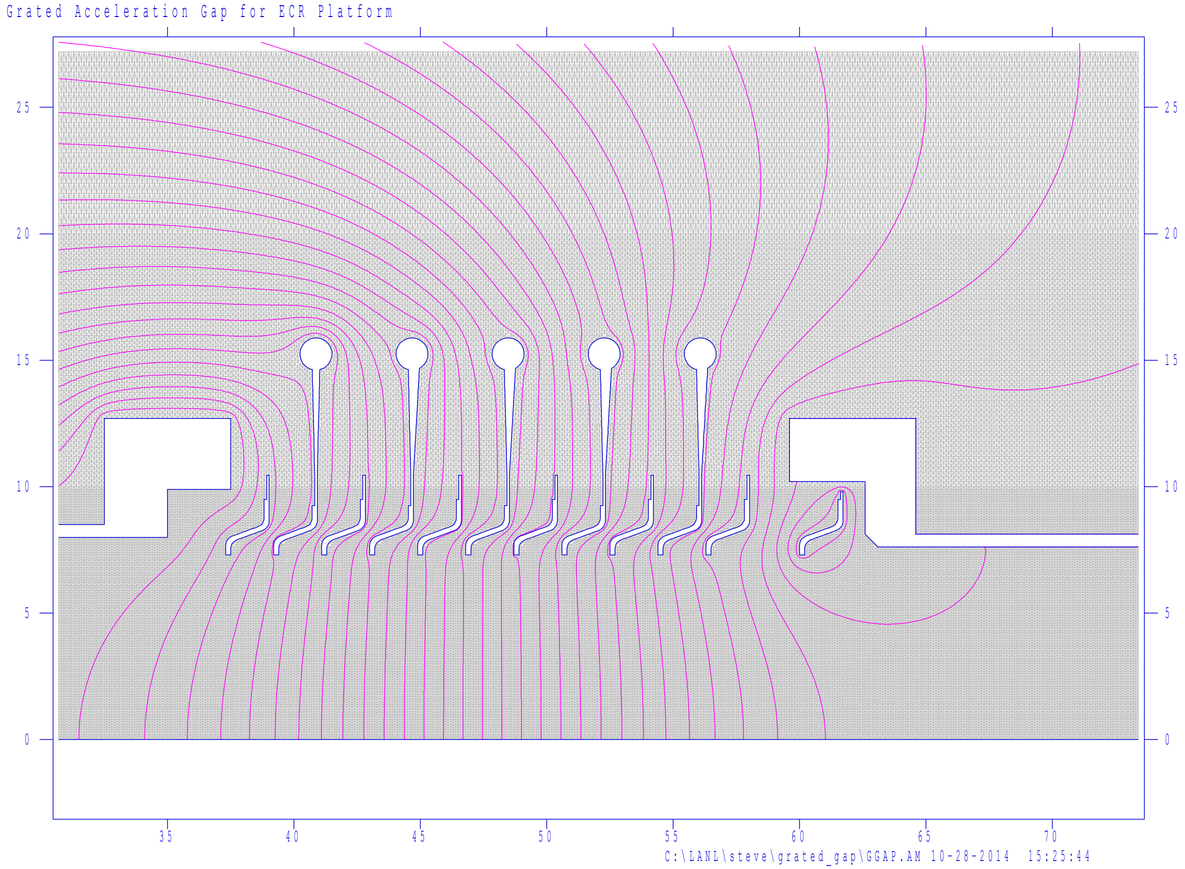


Models imported in high detail from optics design codes Poisson (r-z mesh) and CST Studio

Lattice element model: Grated Electrostatic Accel Gap

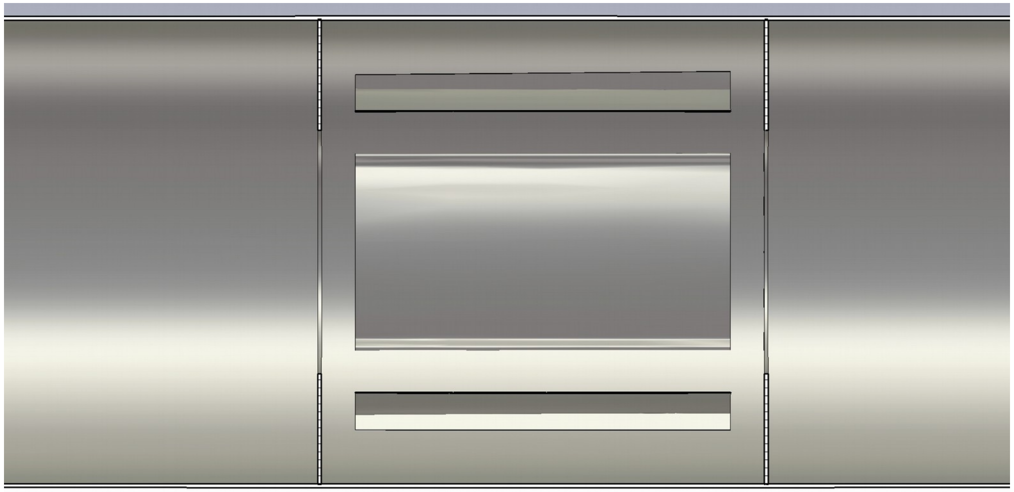
Nonlinear r-z Poisson Model

- » Fringe well resolved
- » Downstream electron suppressor electrode included



Lattice element model: Electrostatic quadrupoles

Cross Section



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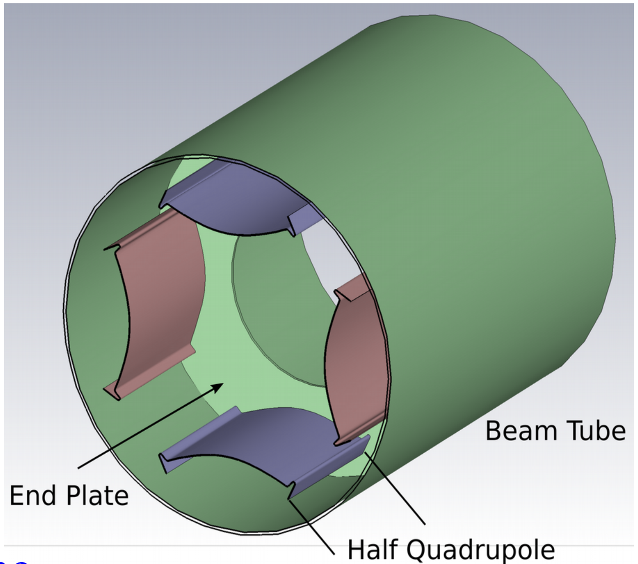
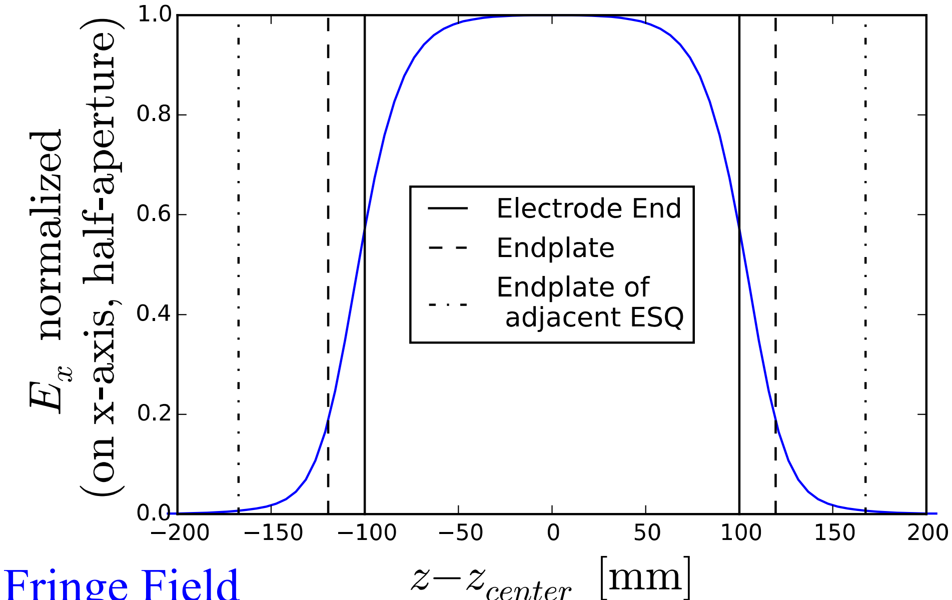
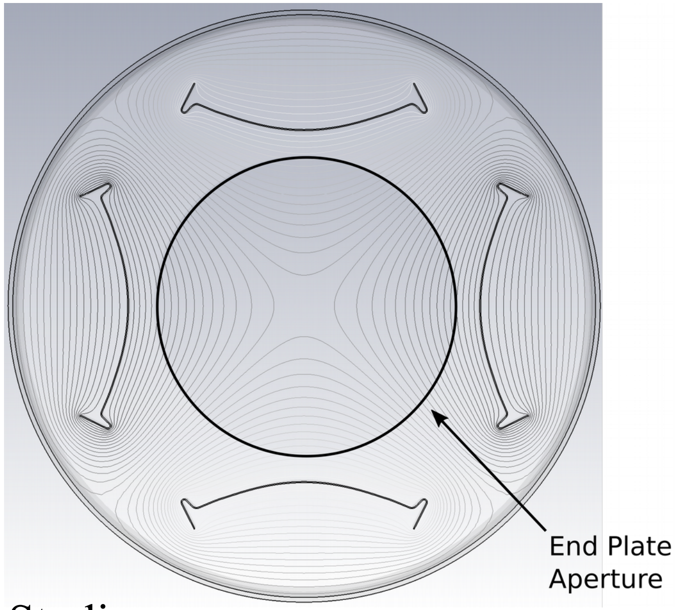




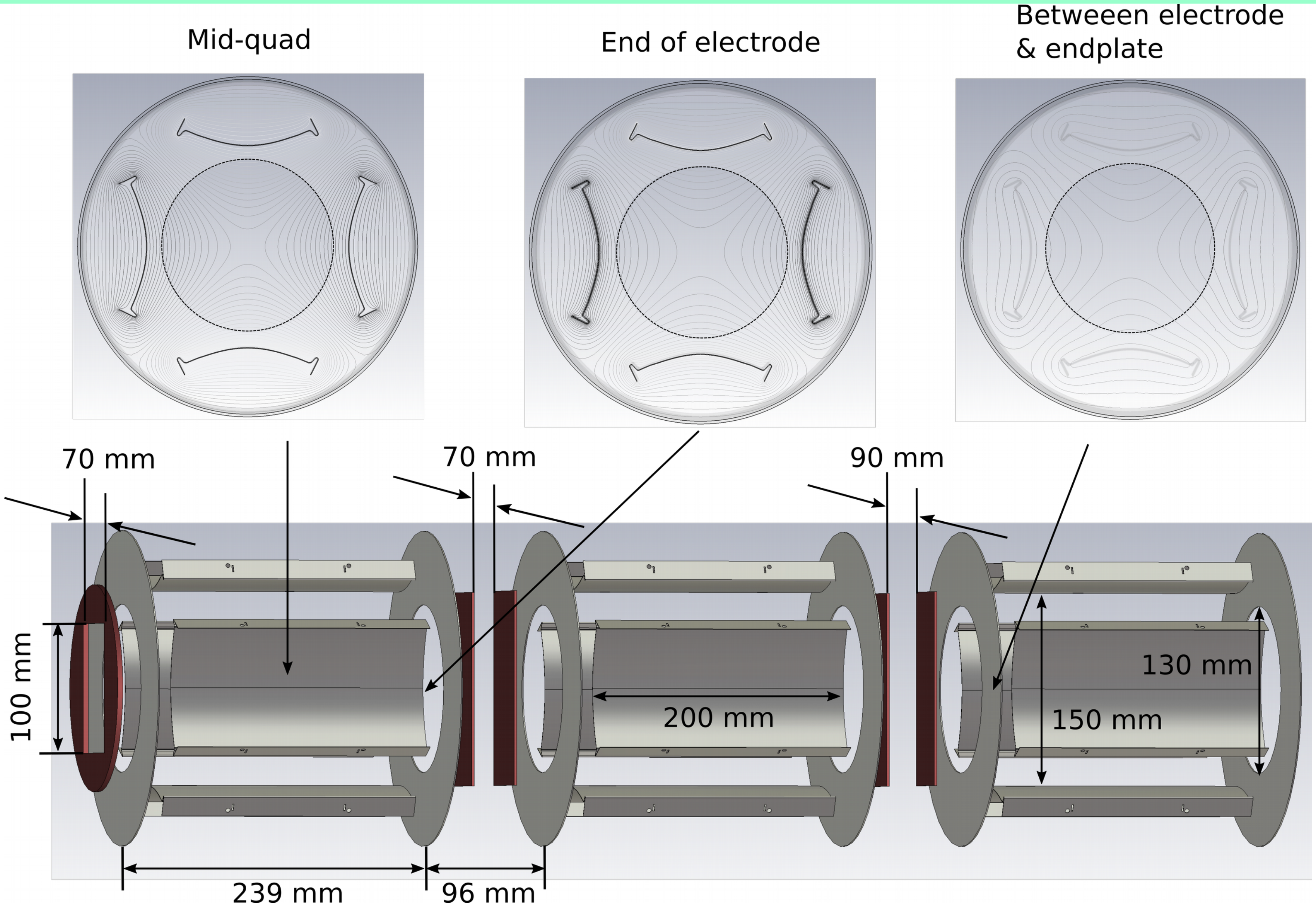
Fringe Field
(Perp Gradient)

Mid-Plane
Potential
Contours



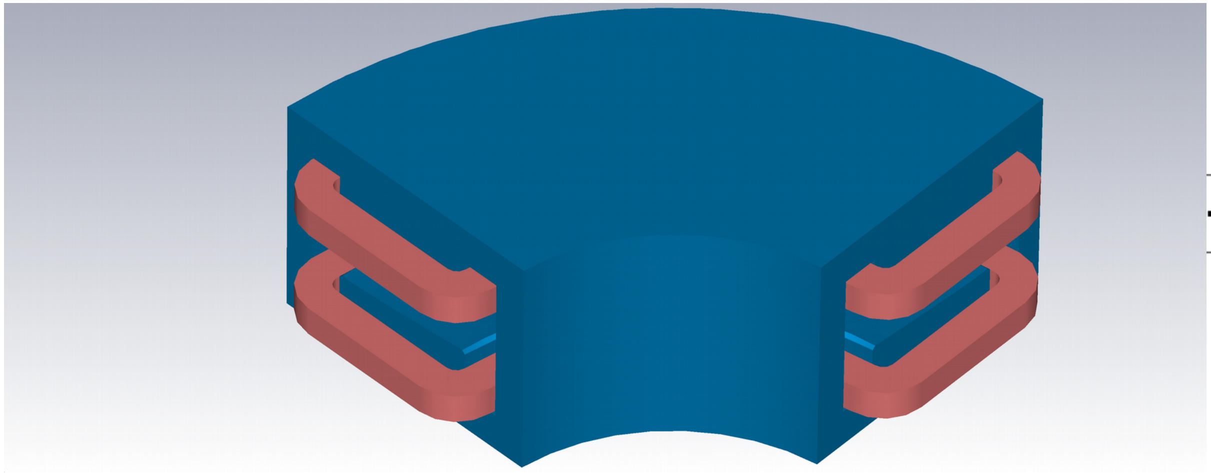
Models imported from CST Studio

Lattice element model: Electrostatic quadrupoles and collimation electrodes

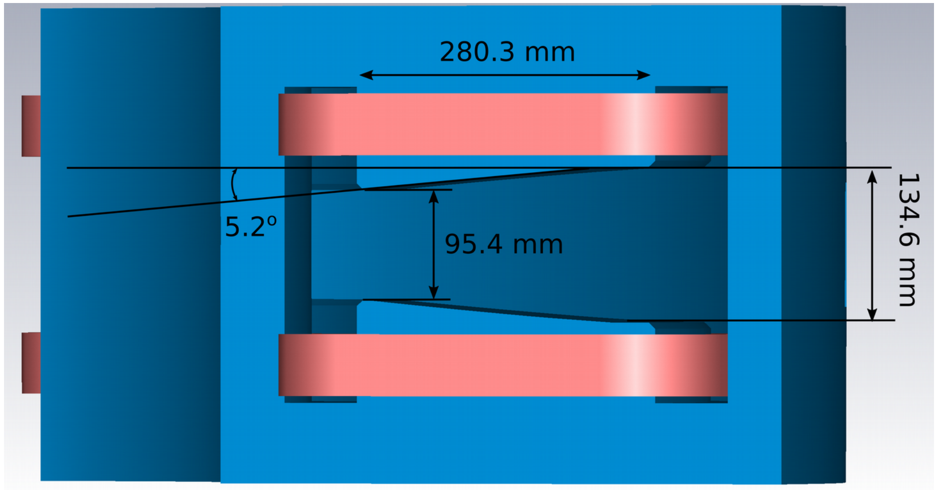


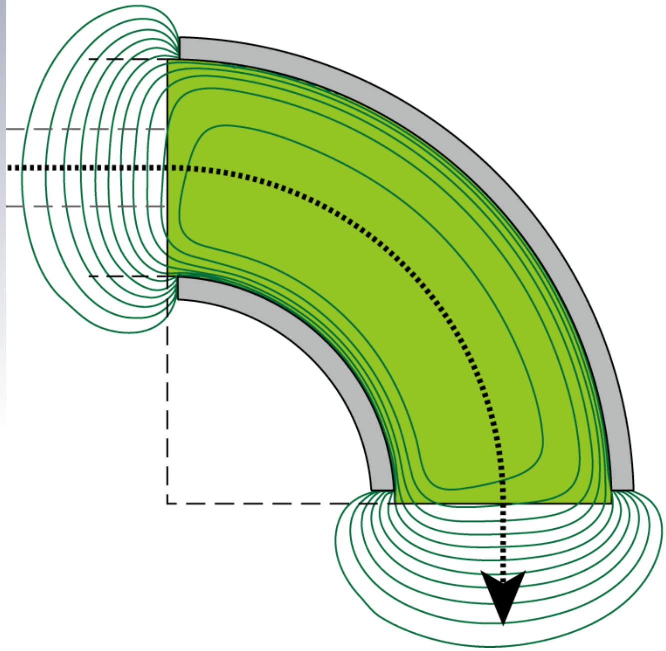
Lattice element model: Magnetic bending dipole with slanted poles

Perspective View



End View Illustrating Slanted Poles





Dipole Fields modeled in 3D using:

- Opera
- CST Studio

Properties of idealized initial distribution expected from ECR also incorporated: Example ^{238}U

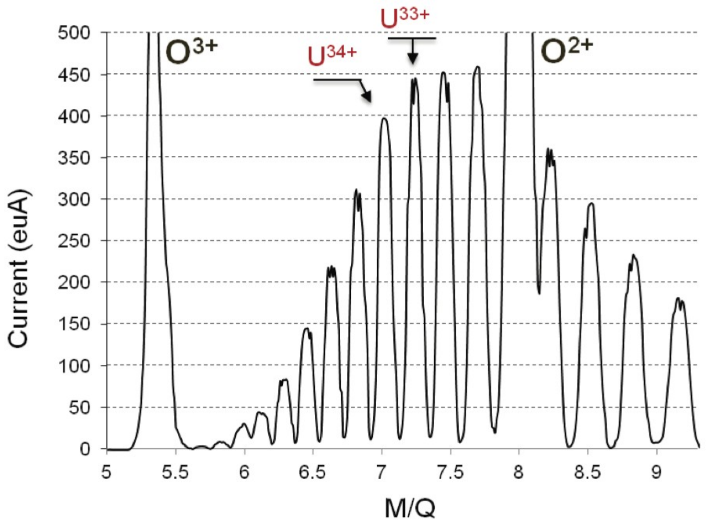
Ion	I (emA)	Q/A	$[B\rho]$ (Telsa-m)
U^{+25}	0.035	0.105	0.0831
U^{+26}	0.051	0.109	0.0815
U^{+27}	0.068	0.113	0.0800
U^{+28}	0.088	0.118	0.0785
U^{+29}	0.115	0.122	0.0772
U^{+30}	0.150	0.126	0.0759
U^{+31}	0.175	0.130	0.0746
U^{+32}	0.192	0.134	0.0735
U^{+33}	0.210	0.139	0.0723
U^{+34}	0.205	0.143	0.0713
U^{+35}	0.178	0.147	0.0702
U^{+36}	0.142	0.151	0.0693
U^{+37}	0.11	0.155	0.0683
U^{+38}	0.072	0.160	0.0674
U^{+39}	0.043	0.163	0.0665
U^{+40}	0.031	0.168	0.0657
O^{+1}	0.3	0.063	0.1077
O^{+2}	0.3	0.125	0.0762
O^{+3}	0.3	0.188	0.0622
O^{+4}	0.2	0.250	0.0539

Target Species (U^{+33}, U^{+34})

Many species possible

- Uranium most rigid
- Rigidity:

$$[B\rho] = \frac{\gamma\beta mc}{q}$$



Initial phase-Space areas set consistently with magnetized ions born in source: Multi-species envelope equation for Gaussian distributed radial charge densities helps setup

$\sigma_{rj} \equiv \sqrt{\langle r^2 \rangle_j}$ rms radius, jth species $\langle \cdots \rangle_j$ average wrt jth species

$$\sigma''_{rj} - \frac{q_j V'}{2\mathcal{E}_{kj}}\sigma'_{rj} - \frac{q_j V''}{4\mathcal{E}_{kj}}\sigma_{rj} + \left(\frac{q_j B_{z0}}{2m_j \beta_{bj} c}\right)^2 \sigma_{rj} - \sum_{s,\text{species}} Q_{js} f_s \frac{\sigma_{rj}}{\sigma_{rj}^2 + \sigma_{rs}^2} - \frac{\varepsilon_{rj}^{\text{rms }2} + \langle P_\theta \rangle_j^2/(m_j \beta_{bj} c)^2}{\sigma_{rj}^3} = 0$$

Matrix space-charge perveance:
species s impact on jth species

$$Q_{js} = \frac{q_j I_s}{2\pi\epsilon_0 m_j \beta_{bj}^2 \beta_{bs} c^3}$$

Contrast:
Single Species $Q = \frac{qI}{2\pi\epsilon_0 m \beta_b^3 c^3}$

Neutralization fraction: $f_j \in [0, 1]$

Species s kinetic energy gain in accel potential:

$$\mathcal{E}_{kj} = \mathcal{E}_{kj}|_{\text{initial}} + q_j [V|_{\text{initial}} - V]$$

$$\beta_{bj} = \sqrt{\frac{2\mathcal{E}_{kj}}{m_j c^2}}$$

$$f_j = \begin{cases} 0, & \text{full neutralized} \\ 1, & \text{unneutralized (bare)} \end{cases}$$

Radial Thermal Emittance

$$\begin{aligned}\varepsilon_{rj}^{\text{rms }2} &= \langle x^2 + y^2\rangle_j \langle x'^2 + y'^2\rangle_j - \langle xx' + yy'\rangle_j^2 - \langle xy' - yx'\rangle_j^2 \\ &= 4\varepsilon_{xj}^{\text{rms }2} - \langle xy' - yx'\rangle_j^2 \quad \text{(Axisymmetric beam only)}\end{aligned}$$

$$\varepsilon_{xj}^{\text{rms }2} = \langle x^2\rangle_j \langle x'^2\rangle_j - \langle xx'\rangle_j^2$$

$$\varepsilon_{nrj}^{\text{rms}} = \beta_{bj}\varepsilon_{rj}^{\text{rms}} = \text{const for linear forces}$$

Canonical Angular Momentum

$$\frac{\langle P_\theta\rangle_j}{m_j\beta_{bj}c} = \langle xy'\rangle_j - \langle yx'\rangle_j + \frac{q_j B_{z0}}{2m_j\beta_{bj}c}\langle x^2 + y^2\rangle_j \quad = \quad \text{const}$$

$$B_{z0} = B_z(r = 0, z)$$

$$\langle P_\theta\rangle_j = \text{const for Linear OR Nonlinear Forces}$$

Total Effective Phase-Space Area

$$\text{Norm. Phase Space Area} = \sqrt{\beta_{bj}^2\varepsilon_{rj}^{\text{rms }2} + \frac{\langle P_\theta\rangle_j}{(m_jc)^2}}$$

Idealized formulas to set Initial ECR Values

Normalized Emittance:

$$\varepsilon_{nrj}^{\text{rms}} = \sqrt{\left(\frac{T_j}{m_j c^2}\right)} R_j$$

$T_j = \text{Temp (Energy Units) jth Species Ion}$

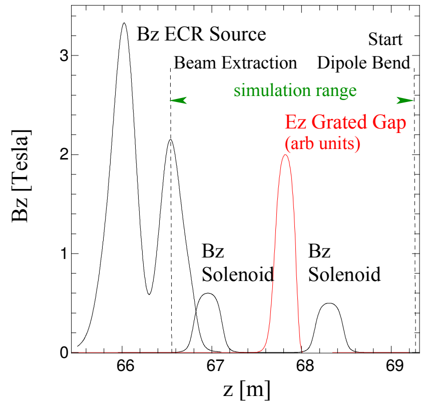
$R_j = \text{Edge Radius jth Species (Uniform Density)}$

$$\varepsilon_{nrj}^{\text{rms}} = \sqrt{\left(\frac{T_j}{m_j c^2}\right)} R_j \sim 0.015 \text{ mm-mrad}$$

Uranium 34+ emerging from ECR

$R_j = 4 \text{ mm}$ beam edge radius

$T_j = 3 \text{ eV}$



Normalized Canonical Angular Momentum:

$$\frac{\langle P_\theta \rangle_j}{m_j c} = \frac{q_j B_{z0}}{4 m_j c} R_j^2$$

At particle "birth" location:

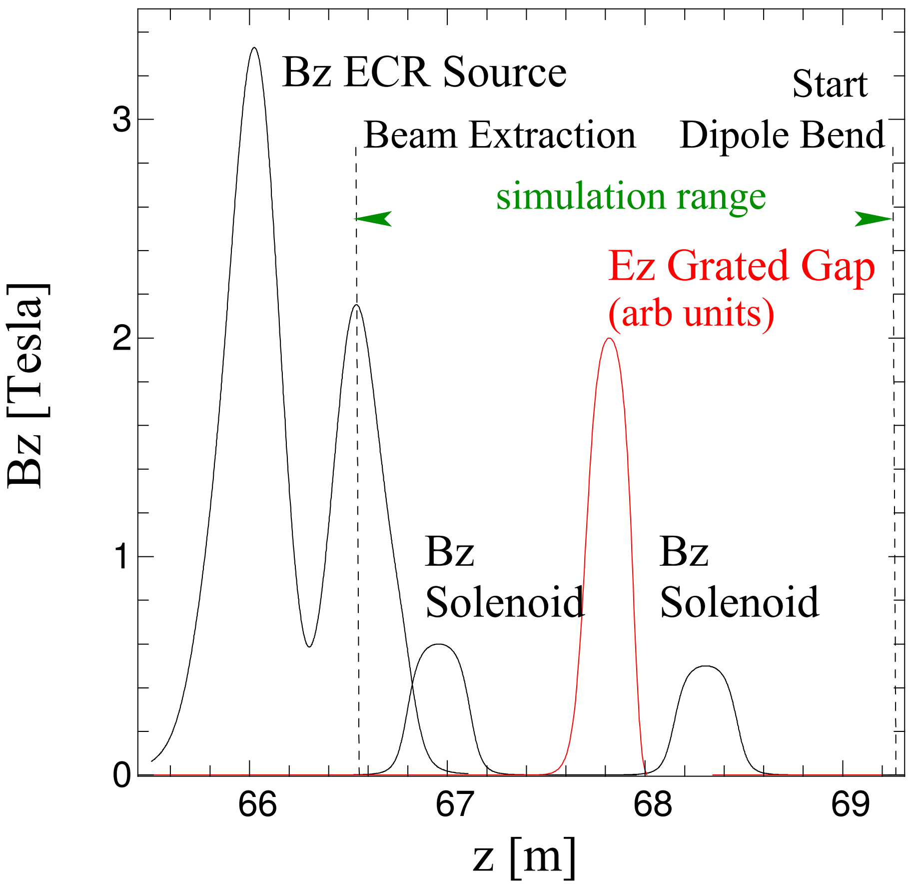
$B_{z0} = B_z(r=0, z) = 2.2 \text{ Tesla (at extraction)}$

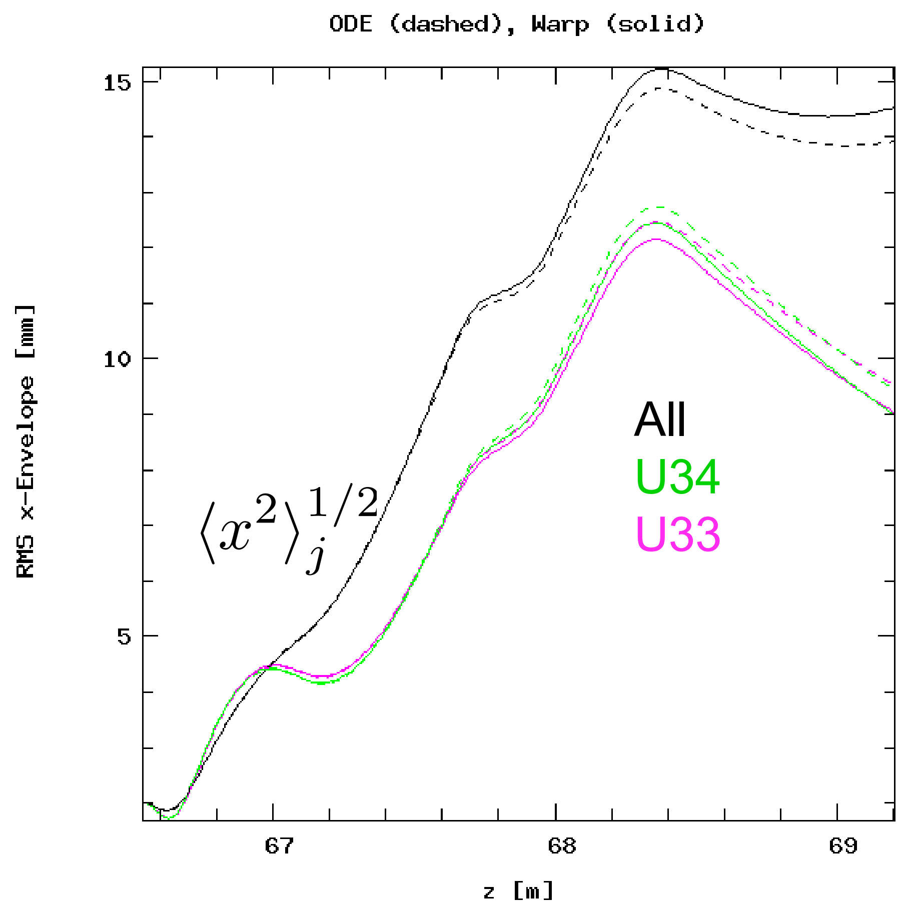
$R_j = \text{Edge Radius jth Species (Uniform Density)}$

$$\frac{\langle P_\theta \rangle_j}{m_j c} = \frac{q_j B_{z0}}{4 m_j c} R_j^2 \sim 0.39 \text{ mm-mrad}$$

~ 25 x Thermal Emittance contribution to phase-space area defocusing!

Comparison to PIC simulations supports that the correct phase-space area measures identified



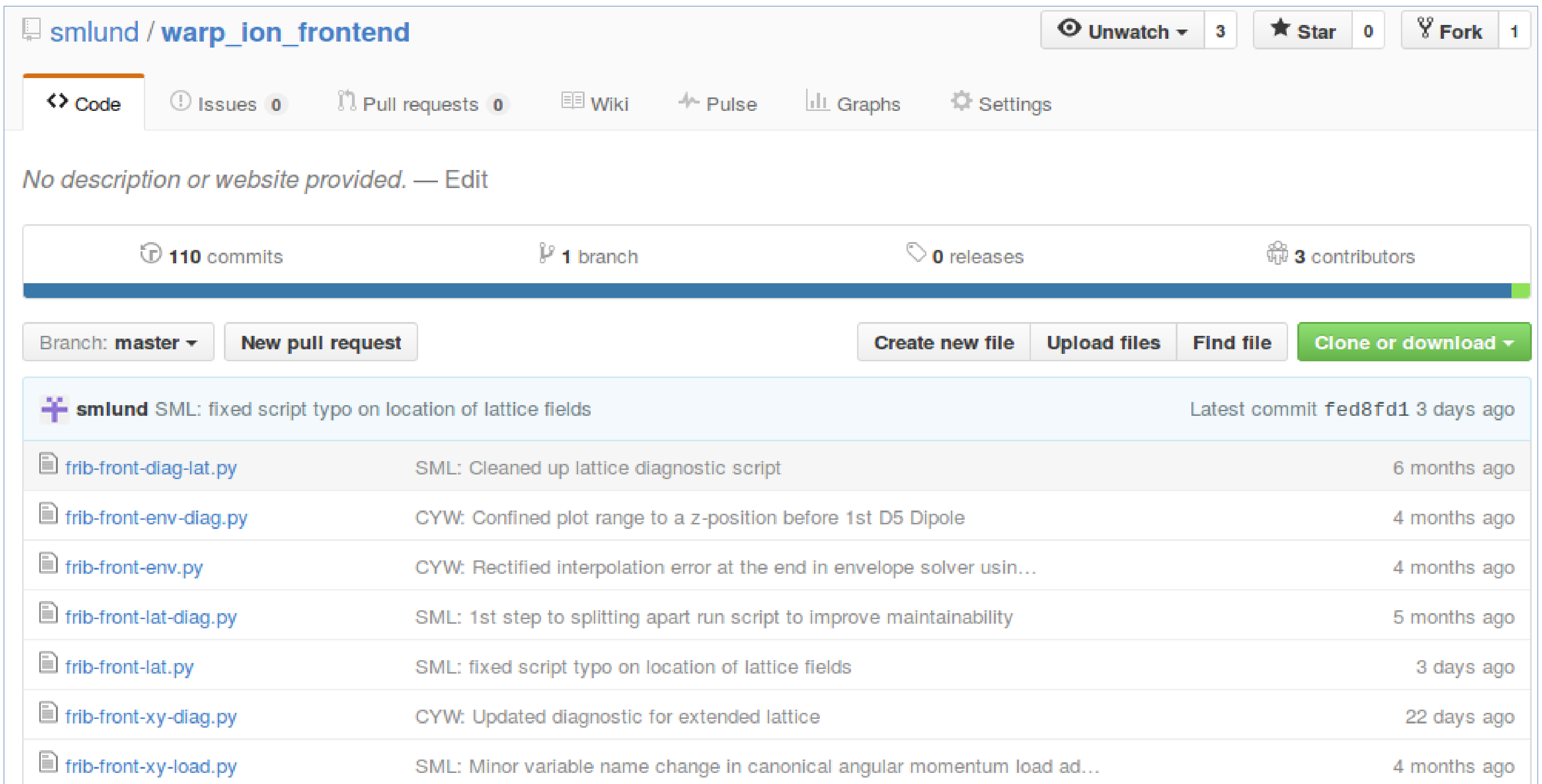


Details of Model: Lund et al, Proc of HB 2014

Warp code tools for front ends setup for maintainability/extension while analyzing many ion species under a range of models with multiple users simultaneously using/extending

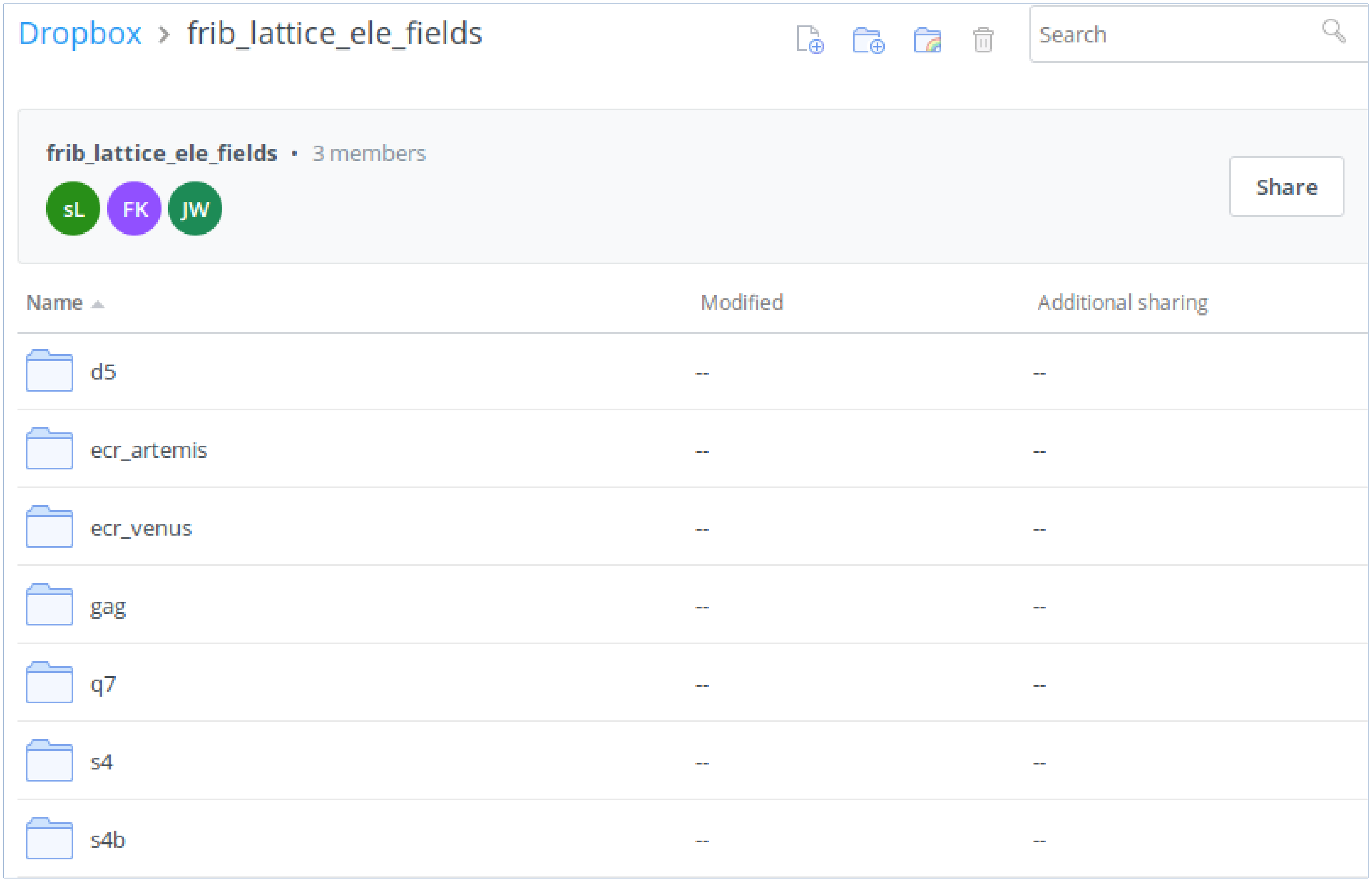
Github source code maintenance used to maintain/distribute python based Warp scripts for front-end simulation and input parameters for runs

- Structured to allow simultaneous users to update/extend while using at same time with different levels of model description
- Allows roll-back, project forking, etc.



Dropbox file sharing used to maintain/distribute field element data for lattice element description

- Works well for large binary/ascii data files on windows/linux/osx platforms
- Archive input, plots, analysis, and code interfaces for each lattice element
- Allows use of links contained in git distribution for data reading without account



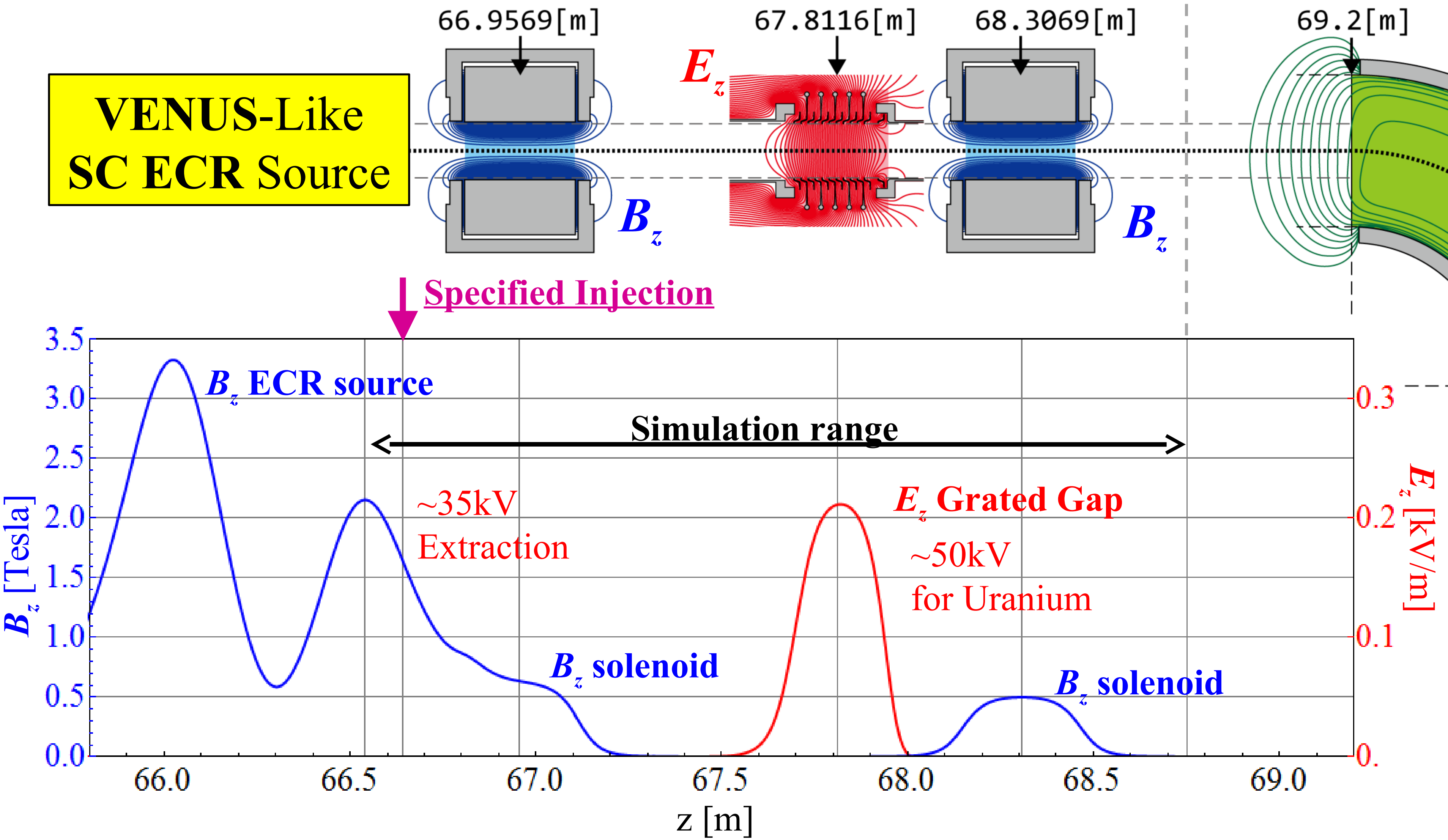
Warp simulations are being applied to the FRIB front end to both identify/analyze physics issues and will be used to support upcoming commissioning activities

Many issues being examined parametrically. Illustrate a few here for ^{238}U:

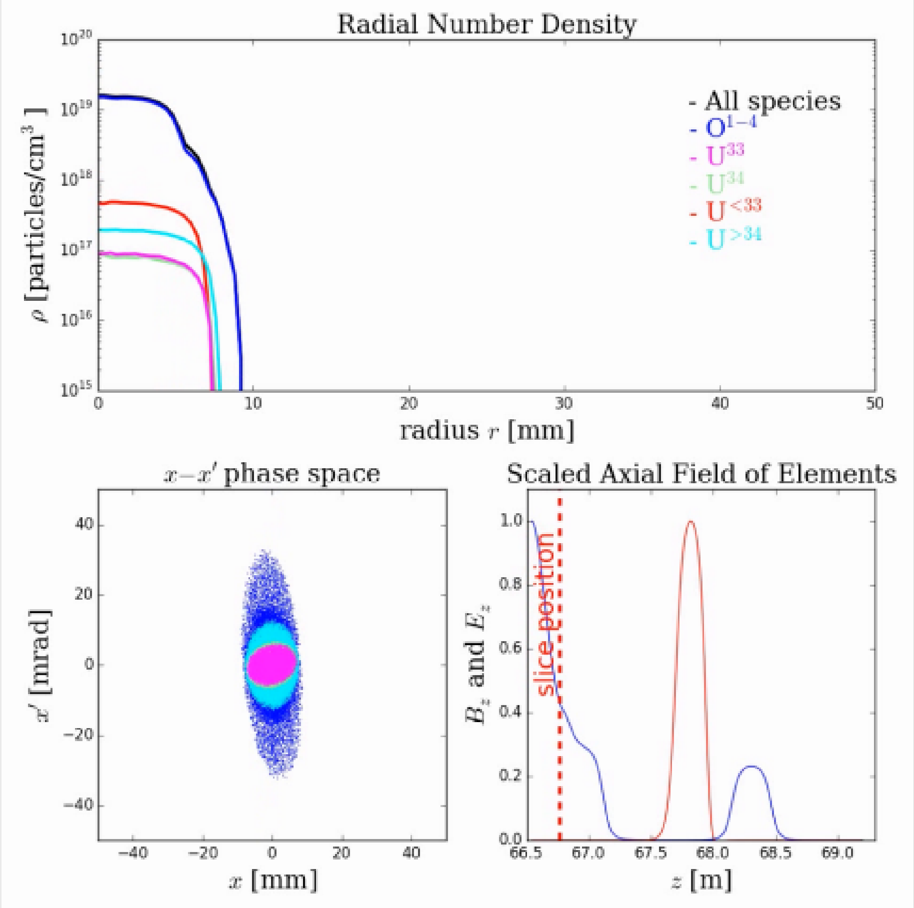
- Multispecies evolution from source with intricate space-charge dynamics
- Optimal placement of 3D dipole with slanted poles
- 3D Space charge effects in initial species separation in dipole

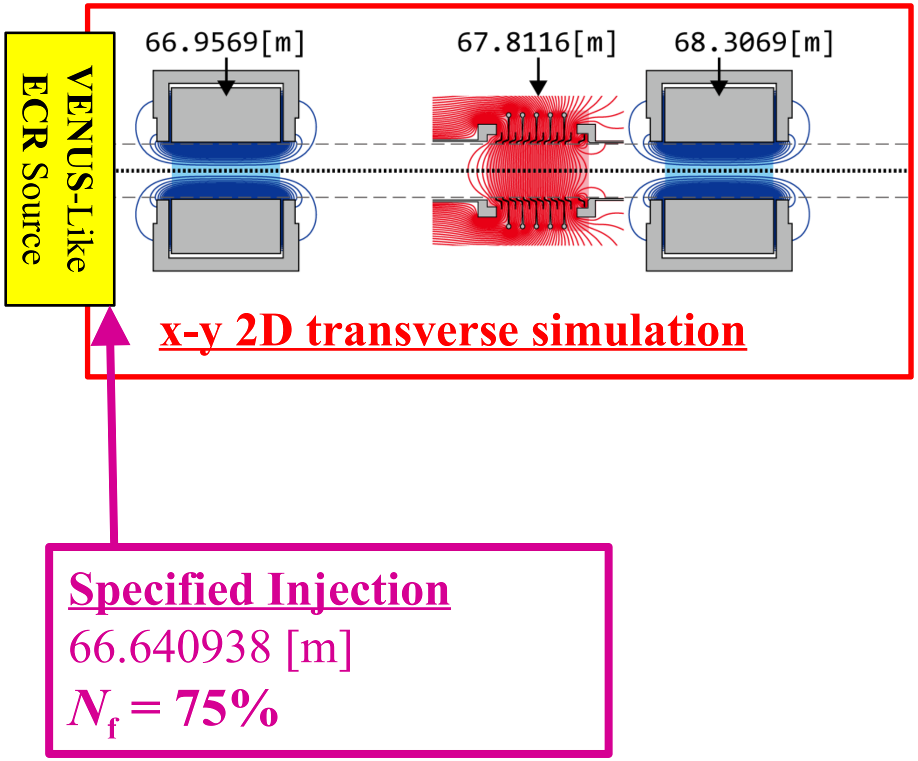
Code can help augment limited laboratory diagnostics to gain more insight and support optimal tuning of system for highest quality beam

Lattice Fields up to 1st Dipole



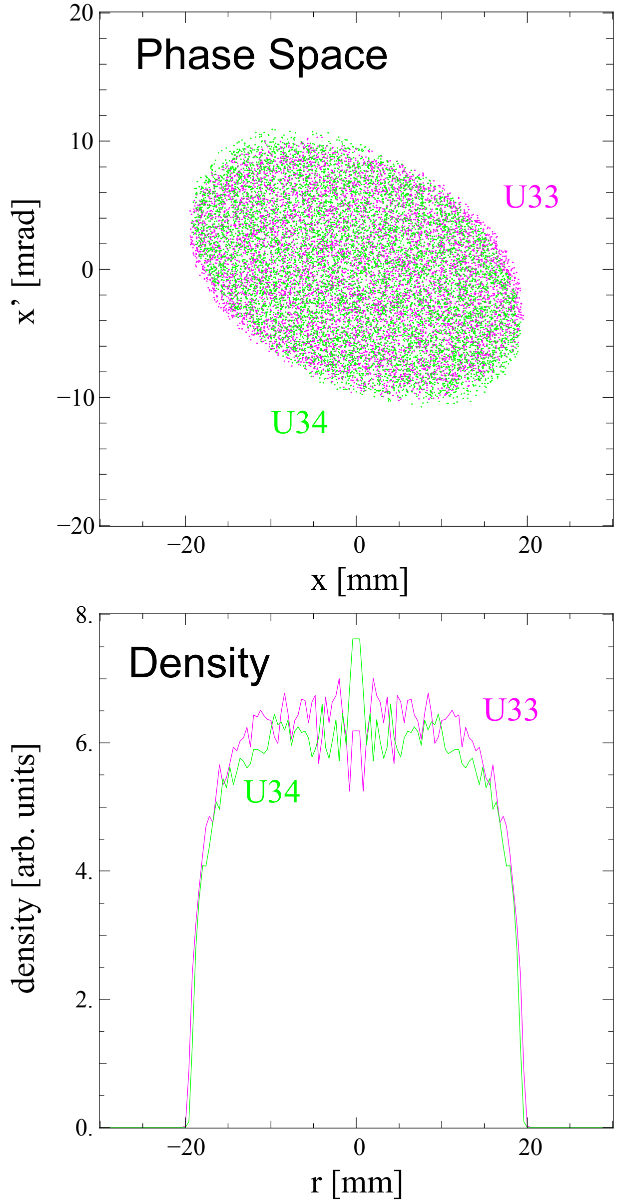
xy-slice simulations of multi-species ion beams emerging from ECR source show little issues in preserving beam quality of target species in spite of intricate phase-space evolution. Movies of correlated phase-space evolution provide insight.



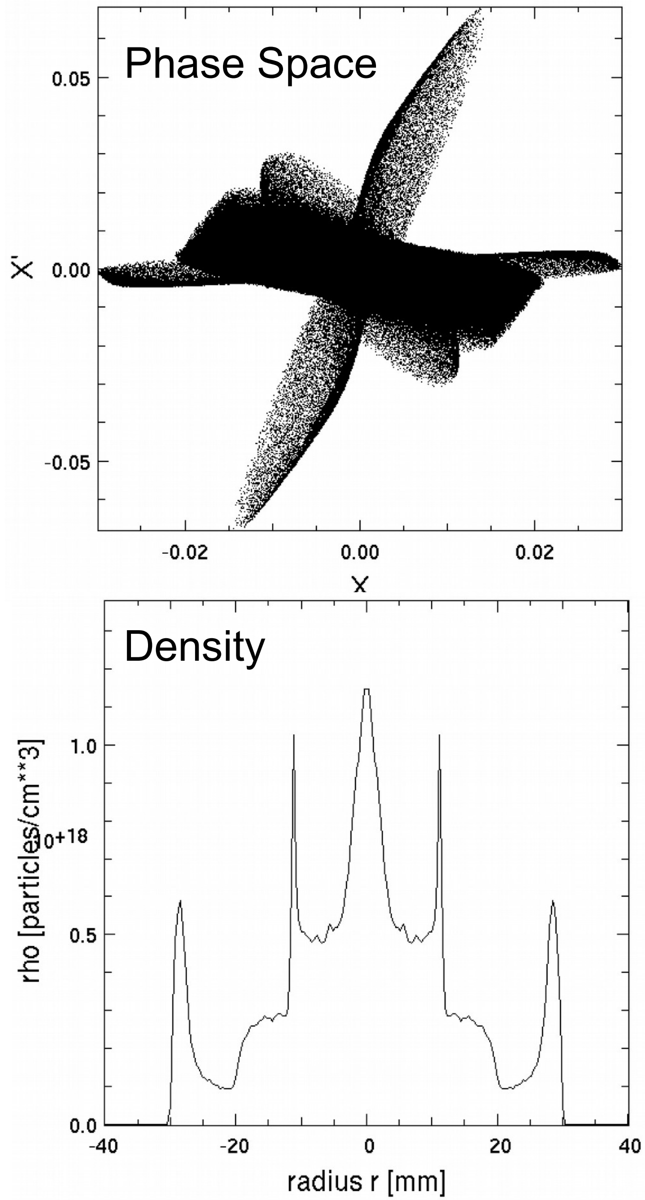


Phase space of target species before dipole shows little distortion over wide range of parameters and operating points

Target Species



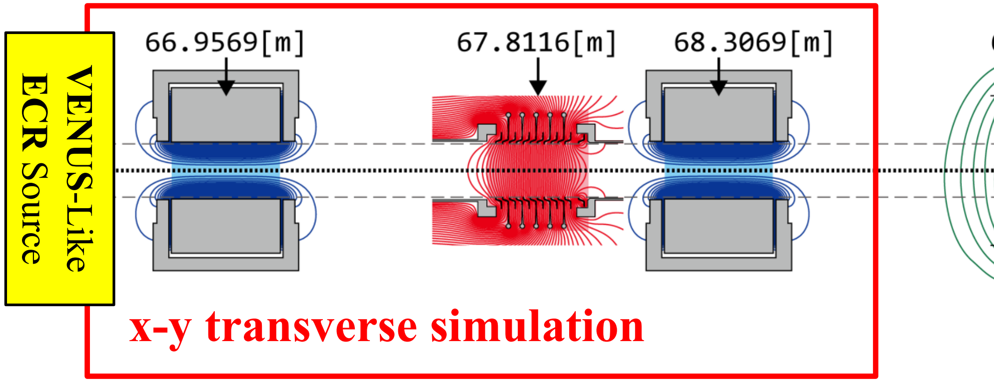
All Species

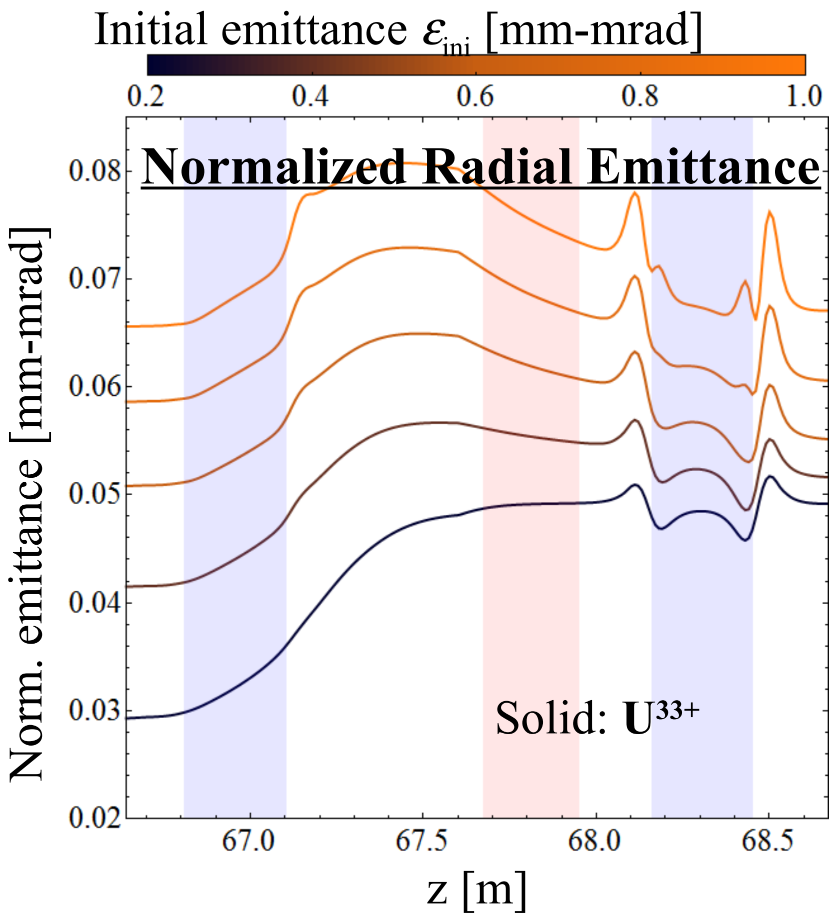


Warp xy slice PIC simulations of first straight section

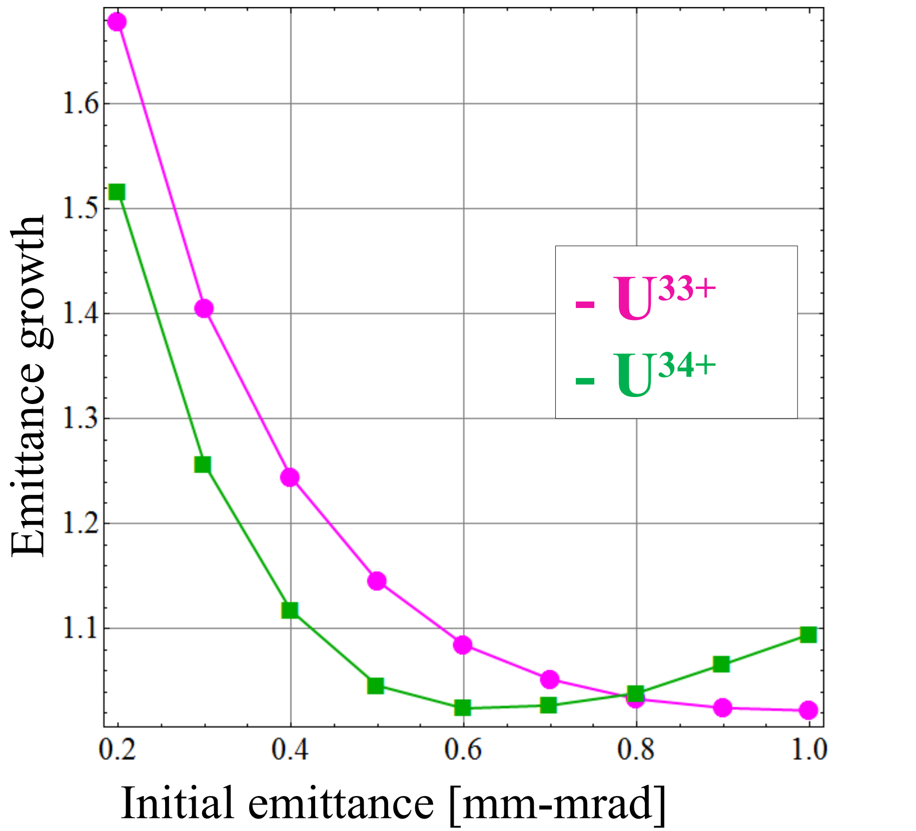
Neutralization factor: 75% (base)

Norm. canonical angler momentum: $\dfrac{P_\theta}{mc} = 0.94759 \times \varepsilon_{\text{ini}}$

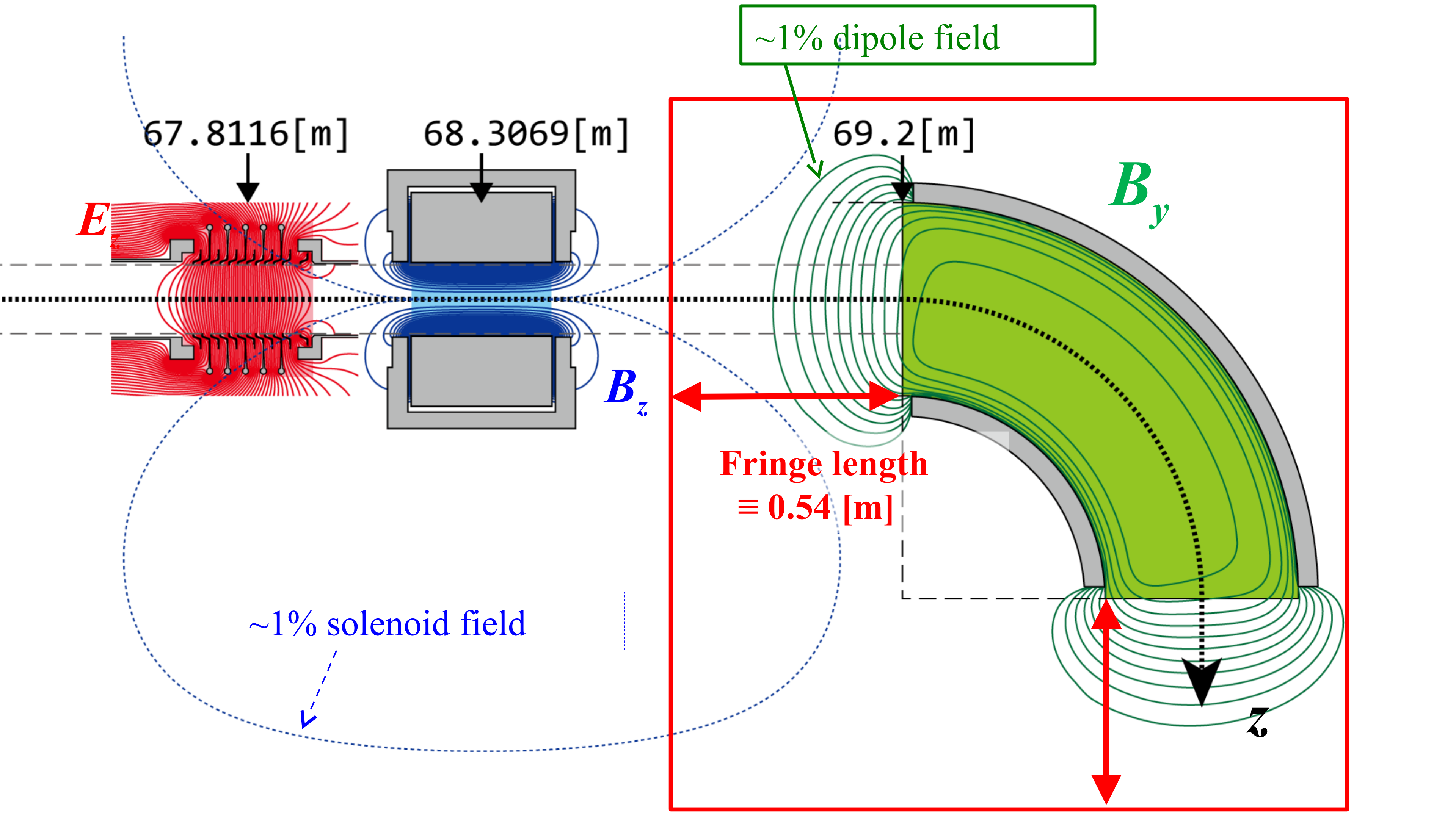




Normalized emittances don't have extent proportional to initial emittance.



Warp 3D PIC simulation with bent grid and 3D dipole field

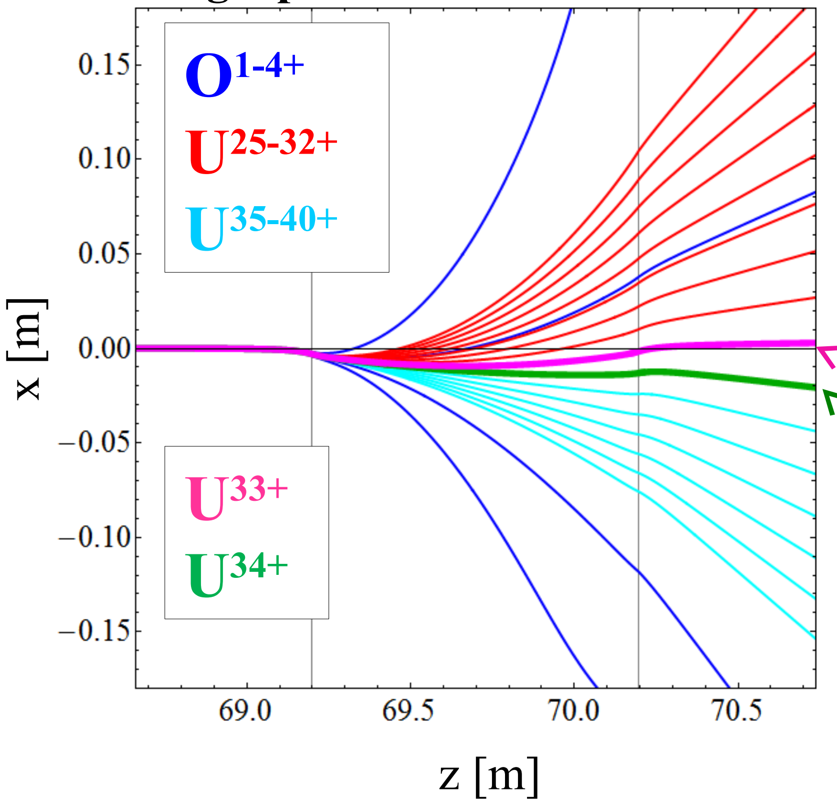


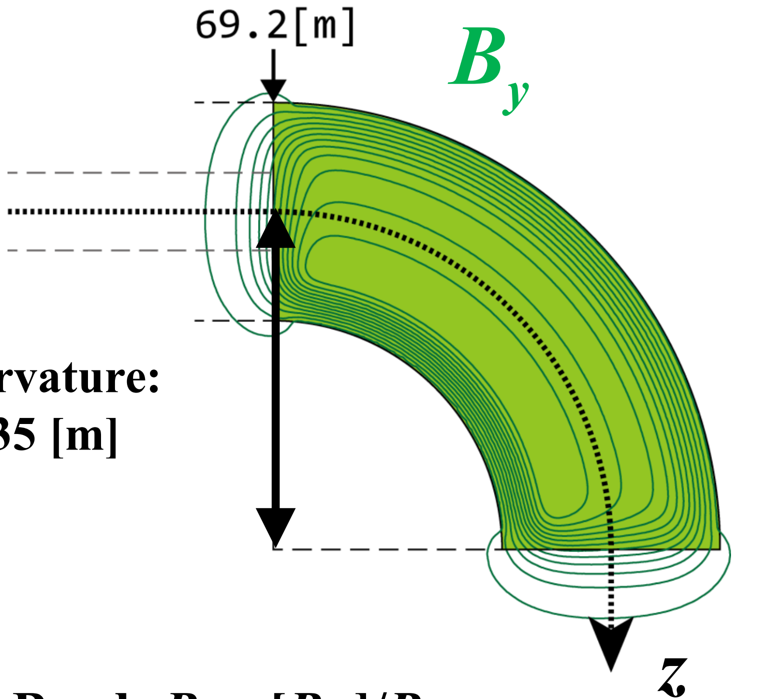
Placement of Real 3D Dipole

3D real dipole
(fringe effect and tapered poles)

Reference orbit **U33**:
$x_{ini}, y_{ini}, vx_{ini}, vy_{ini} = 0.0$

Single particle simulation





Radial curvature:
R = 0.635 [m]

Ideal Bend: $B_y = [B\rho]/R$

Real Bend: Fringe extended and B_y varies over path

U^{33+} x_{fin} = 2.925 [mm]
x'_{fin} = 2.764 [mrad]

U^{34+} x_{fin} =-21.612 [mm]
x'_{fin} =-19.748 [mrad]

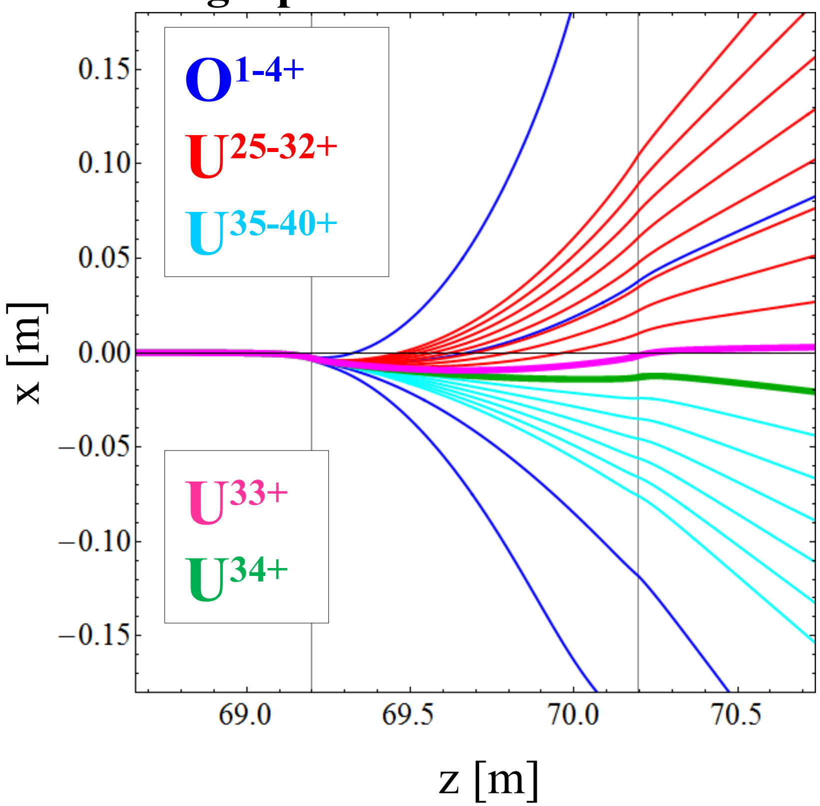
How to Place ?

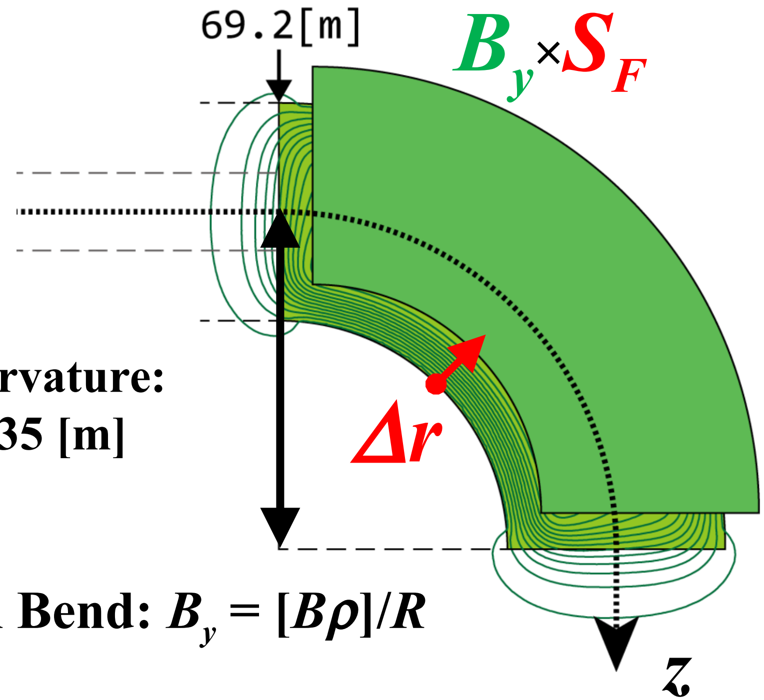
Placement of Real 3D Dipole

3D real dipole
(fringe effect and tapered poles)

Reference orbit **U33**:
x_{ini}, y_{ini}, vx_{ini}, vy_{ini} = 0.0

Single particle simulation





Radial curvature:
R = 0.635 [m]

Ideal Bend: $B_y = [B\rho]/R$

Real Bend: Fringe extended and
B_y varies over path

>> find convergence values by shifting center Δr and scaling field S_F so reference centroid emerges on-axis.

Δr and S_F are solved by numerical root finding with simulation data.

3D Placement Results

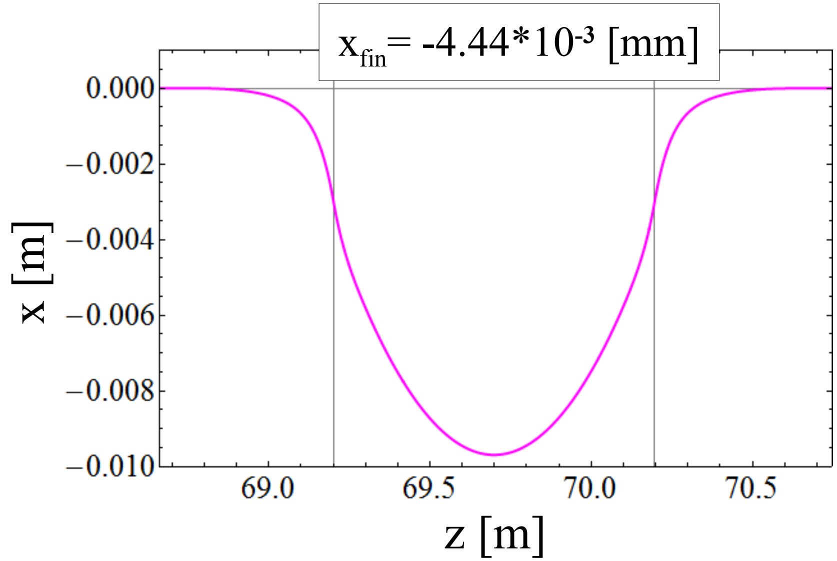
Reference orbit **U33**:

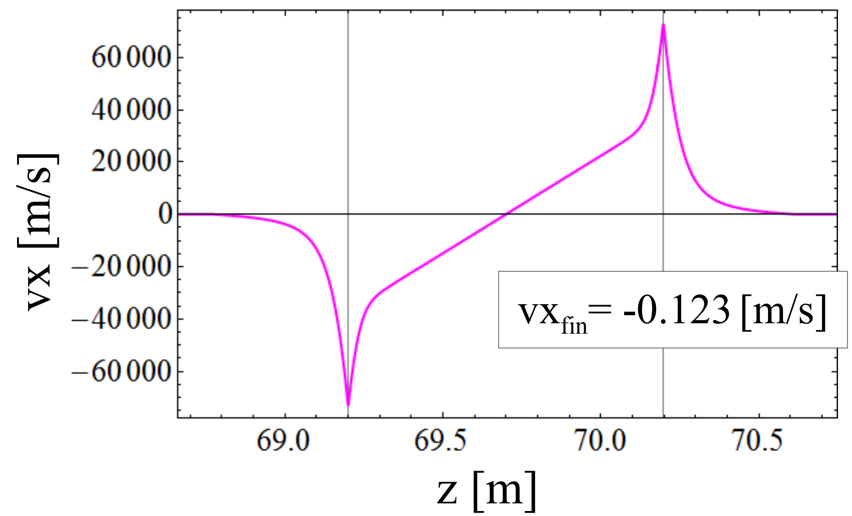
$x_{ini}, y_{ini}, vx_{ini}, vy_{ini} = 0.0$

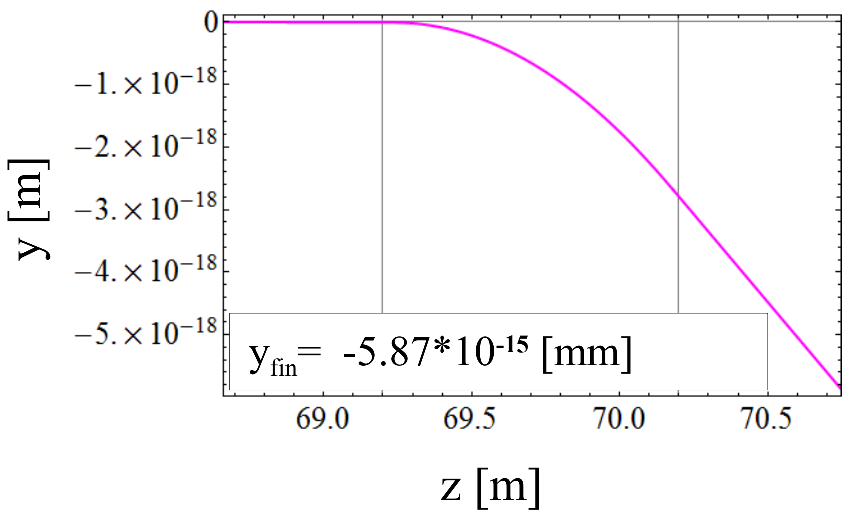
Δr = 1.245×10^{-4} [mm]

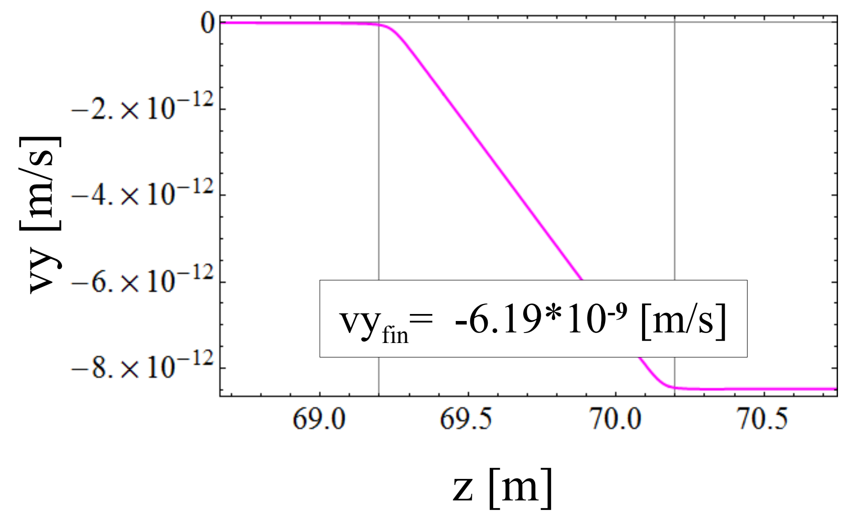
S_F = 1.00185

(relative to ideal dipole)









Summary: Dipole Placement

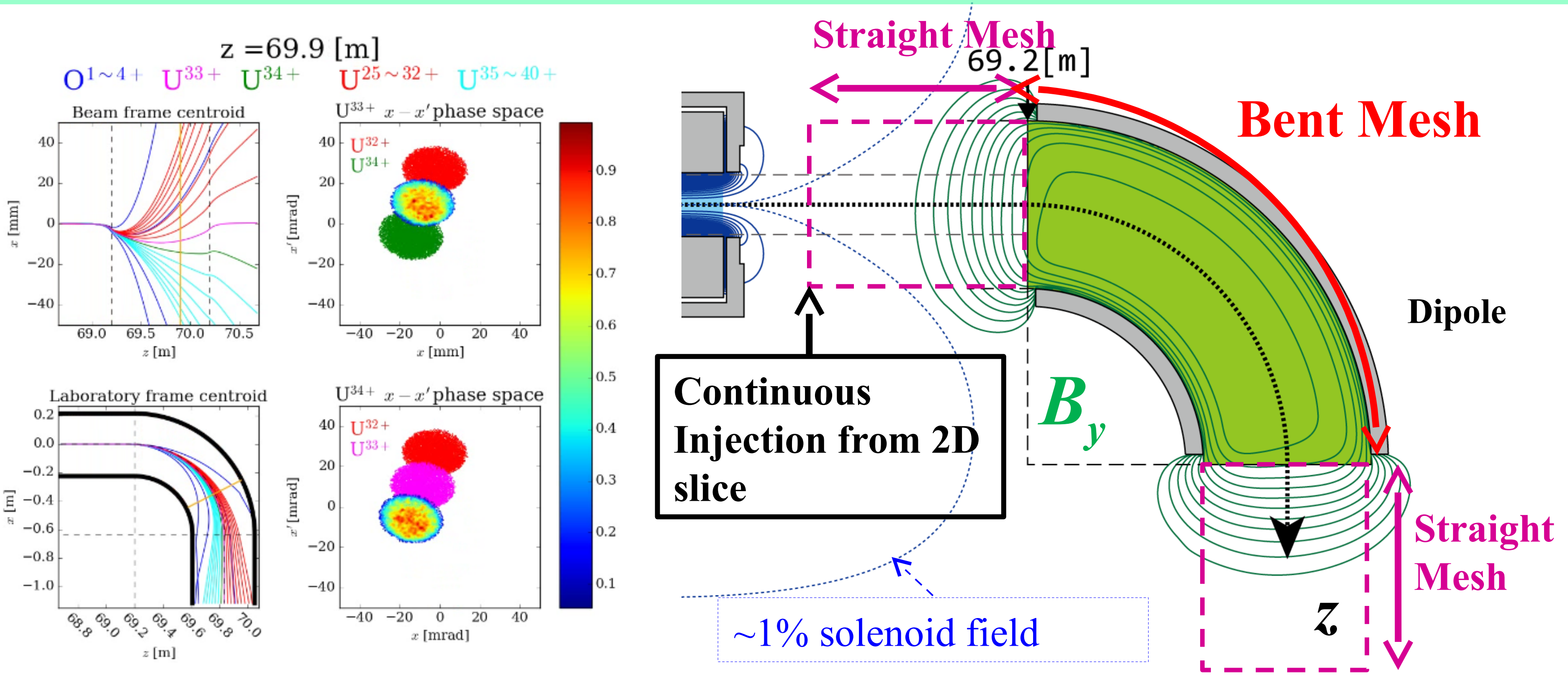
1. Need $\Delta r \sim 0.1$ μm and $\Delta S_F \sim 0.1$ % shift from ideal values for target species to emerge on-axis

   Adjustment from idealized values negligible

2. Solenoid fringe overlap effect negligible

   Fortunate: can adjust placement to compensate when overlap,
   but compensation changes with operating point

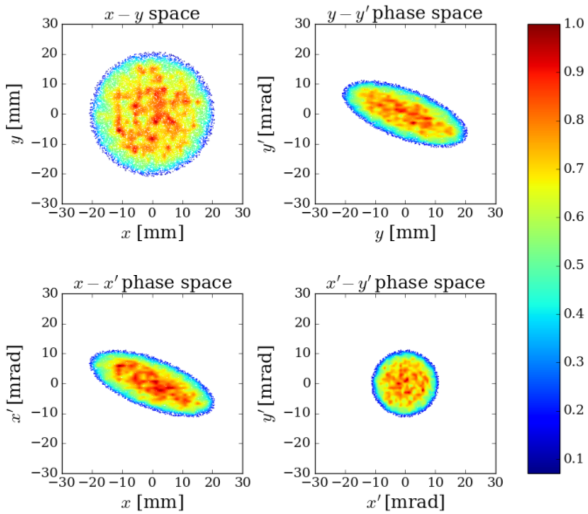
3D simulations of dipole bends with space-charge and full fringe model suggest little issues with beam quality on early species separation



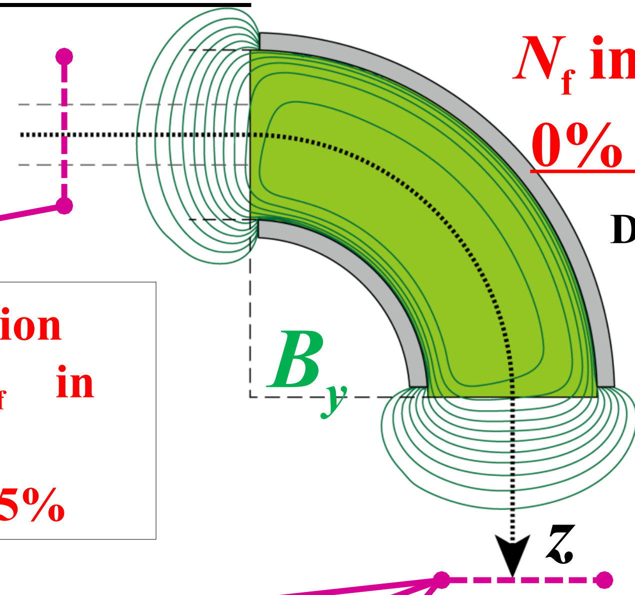
- Injection from 2D slice : numerical "fuzz" added for to continuously inject
- Fringe extends outside of bent mesh adds modeling complications
- Run till steady beam achieved on fixed grid ~ 2 msec filling times (slowest species)

Space-Charge Effect in Real 3D Bend

Initial U33 dist. (z = 68.68 [m])



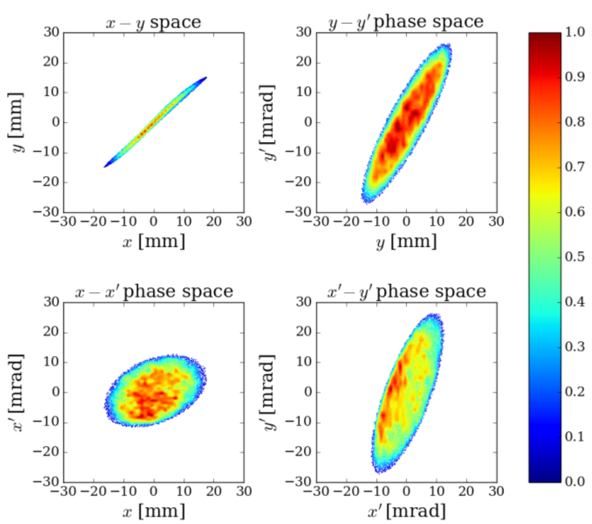
Neutralization factor N_f in straight section = 75%



N_f in bend: 0% ~ 100%

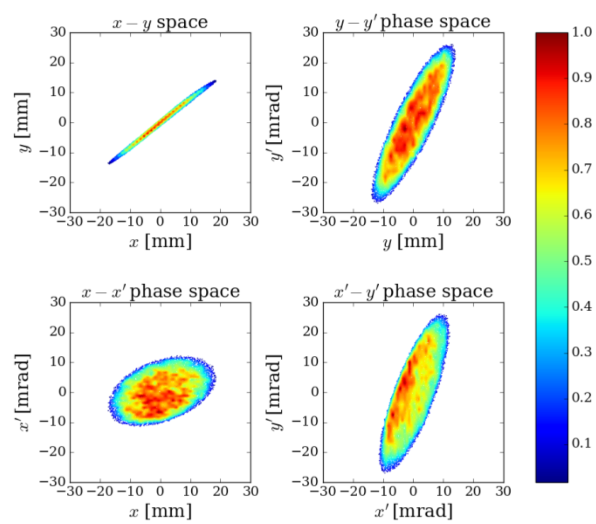
N_f in bend: 100%

U33 at z =70.68 [m]



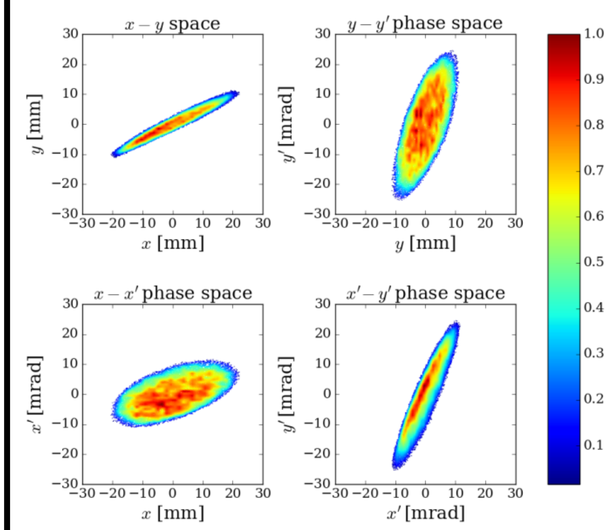
N_f in bend: 75%

U33 at z =70.68 [m]



N_f in bend: 0%

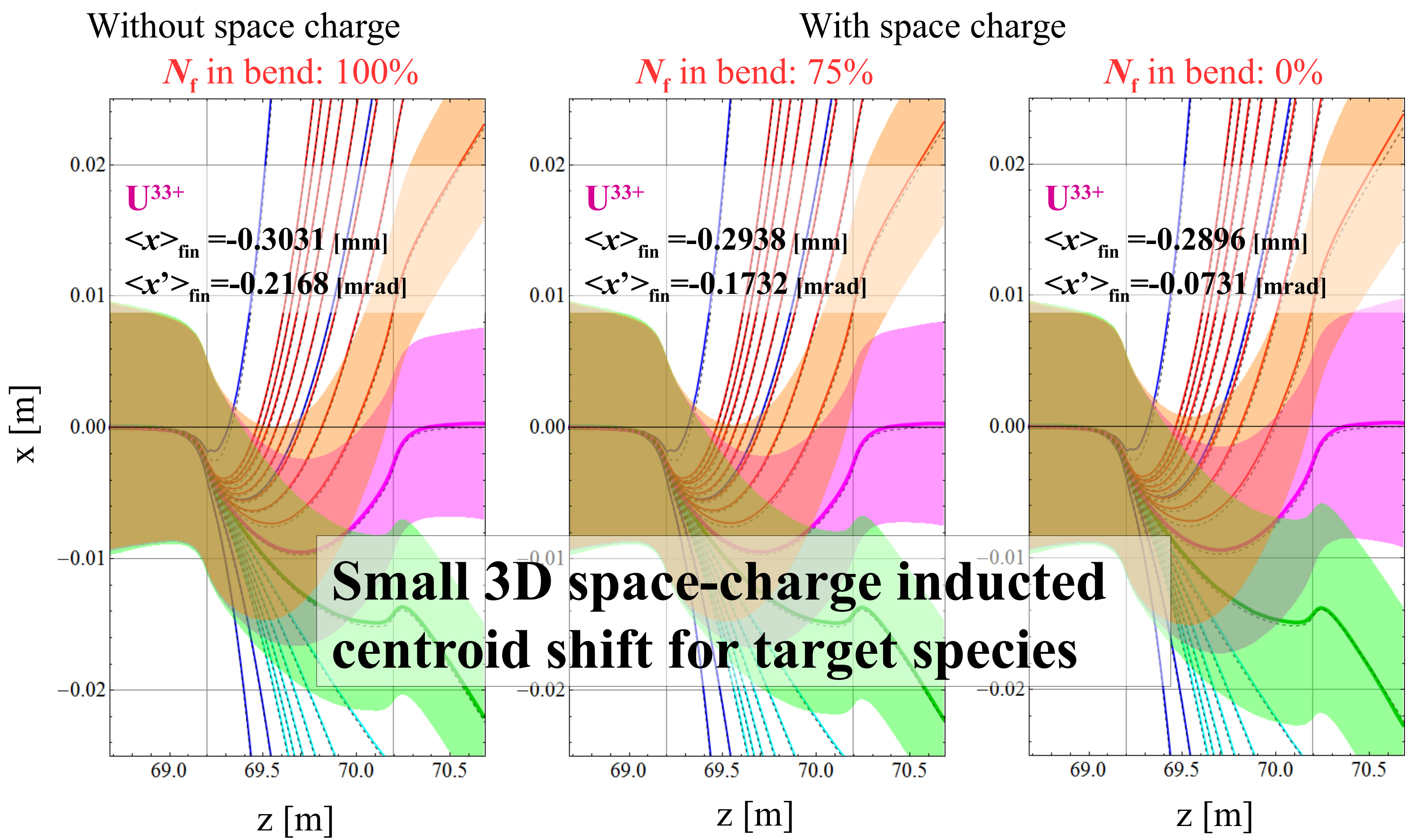
U33 at z =70.68 [m]



Space-Charge Effect in Real 3D Bend

Initialization at z= 68.68 [m] (in front of the bend fringe)

ε_{ini} = 0.4 [mm*mrad], Neutralization factor: N_f = 75%



(black dashed line: single-reference-particle orbit)

Space-Charge Effect in Real 3D Bend

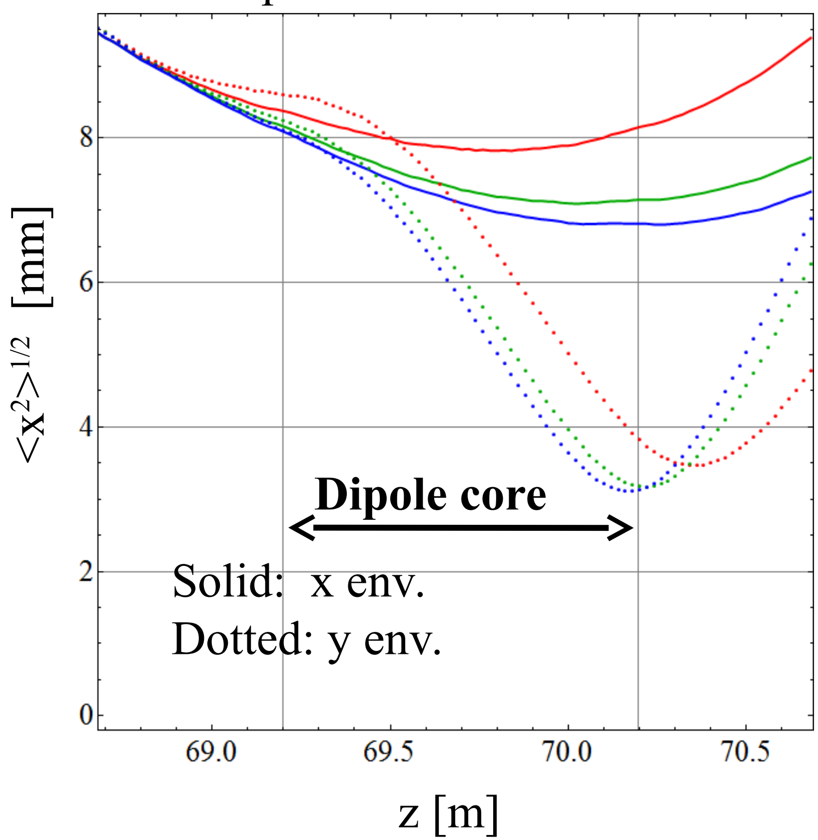
Initialization at z = 68.68 [m] (in front of the bend fringe)

ε_{ini} = 0.4 [mm*mrad], Neutralization factor: N_f = 75%

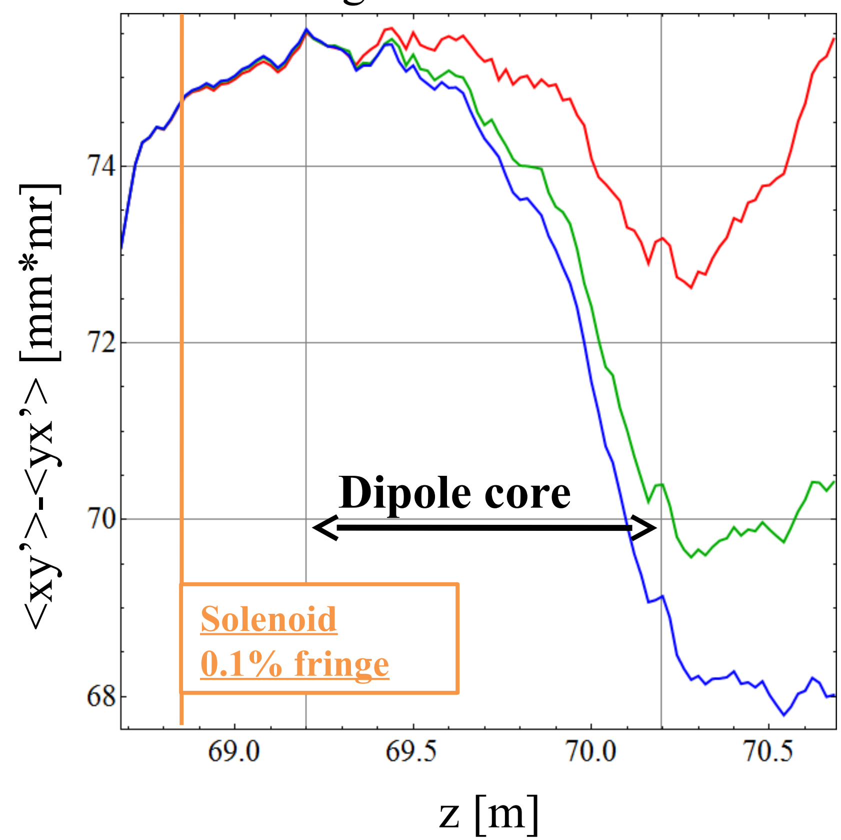
Without space charge — **N_f in bend: 100%**

With space charge — **N_f in bend: 75%** — **N_f in bend: 0%**

Envelope size: **U33**



Mechanical angler momentum: **U33**



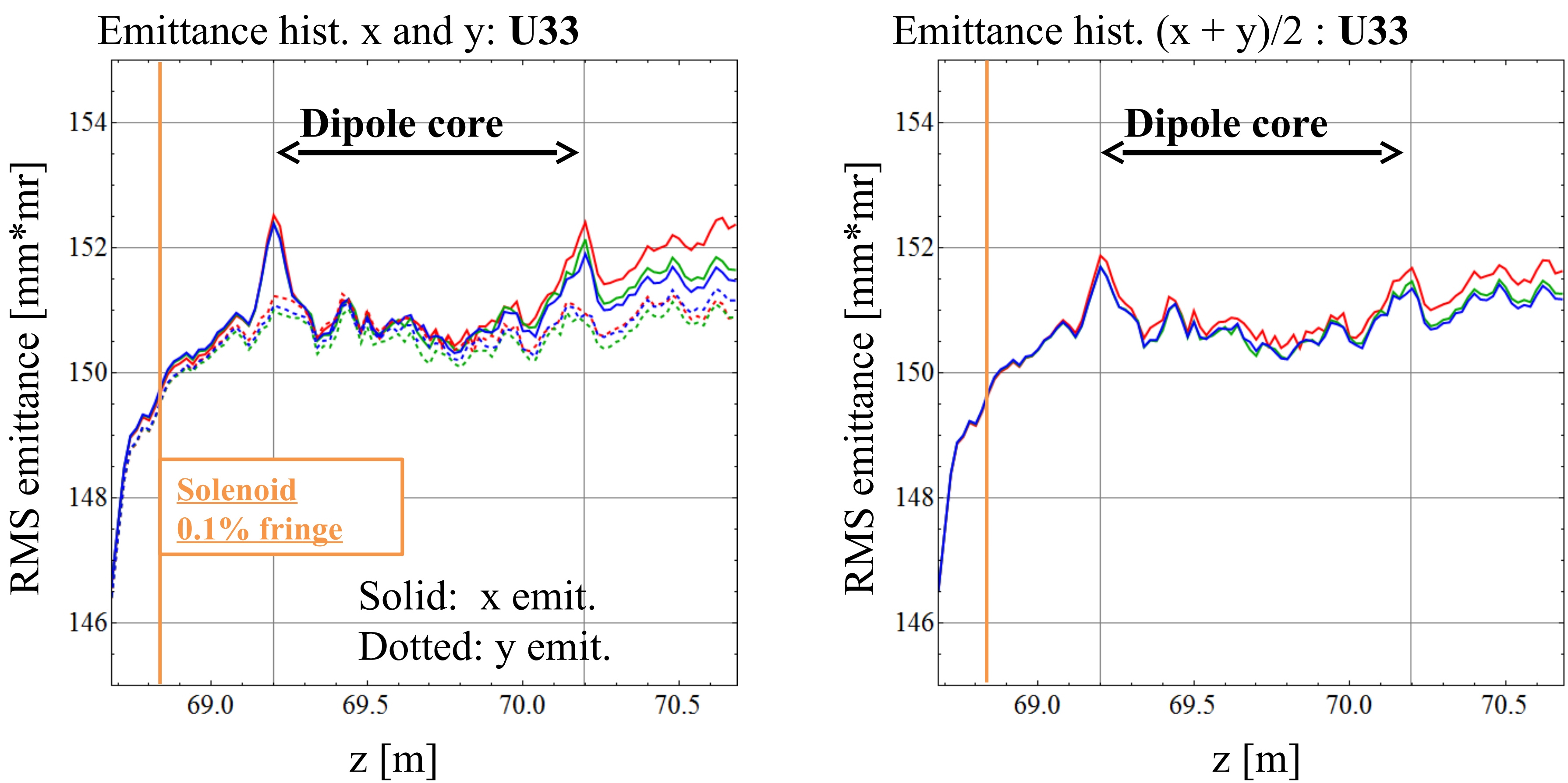
Space-Charge Effect in Real 3D Bend

Initialization at z = 68.68 [m] (in front of the bend fringe)

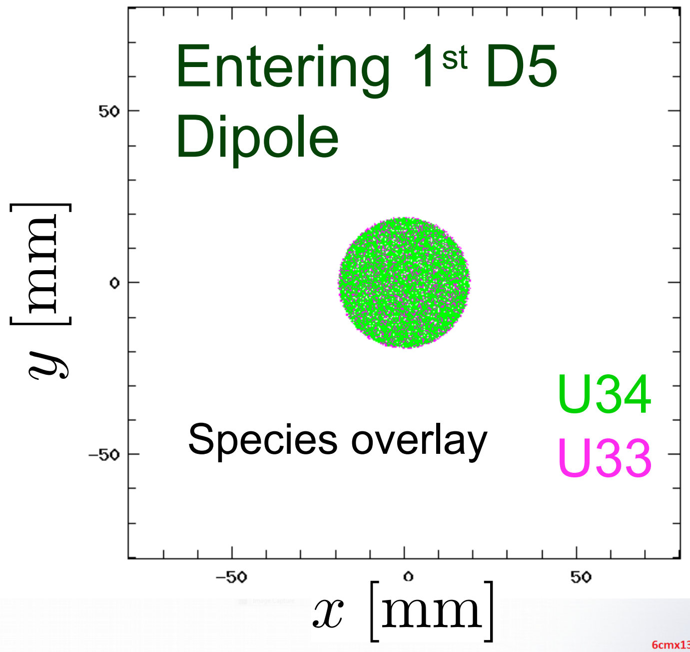
ε_{ini} = 0.4 [mm*mrad], Neutralization factor: N_f = 75%

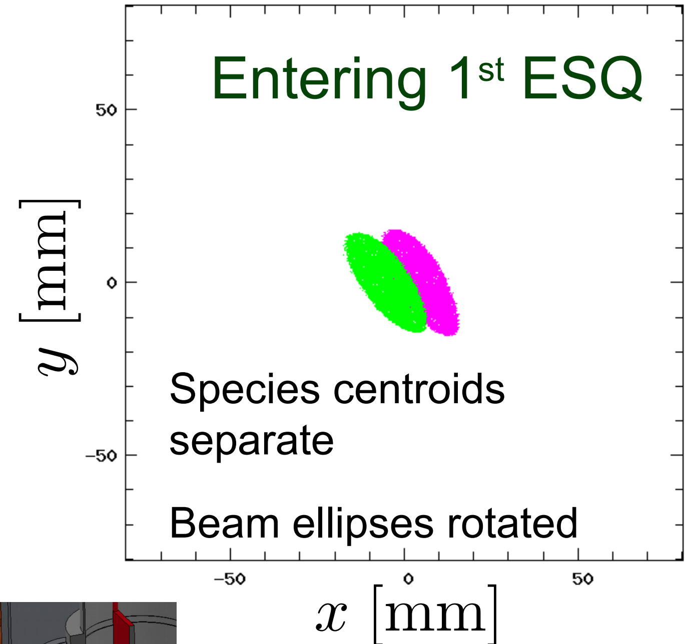
Without space charge | With space charge

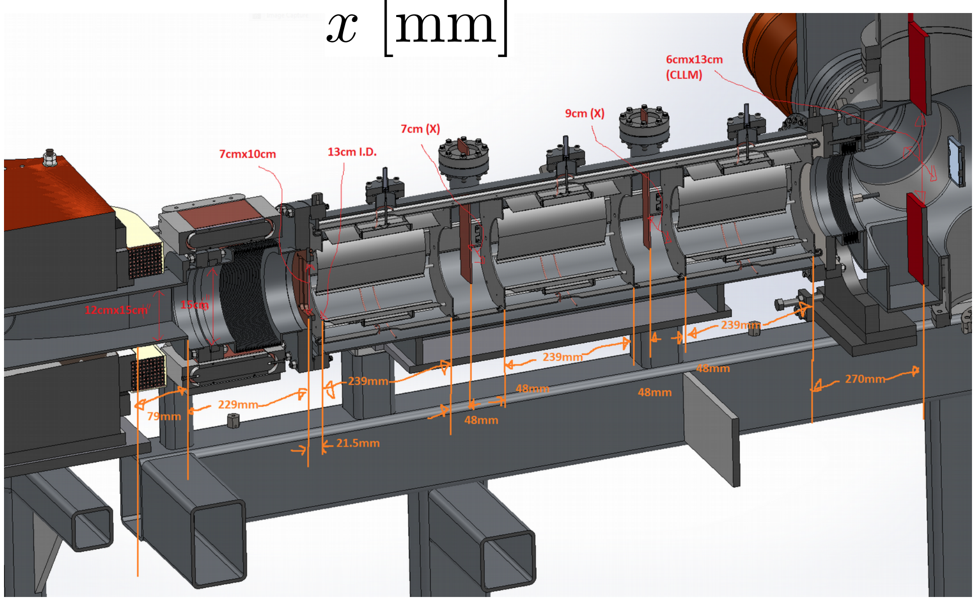
N_f in bend: 100% | **N_f in bend: 75%** | **N_f in bend: 0%**



xy beam becomes tilted in dipole due to (unknown value) of initial canonical momentum $\langle P_\theta \rangle_j$ of beam emerging from ECR. This will complicate optimization of collimation electrodes in ESQs.







Conclusions

Framework for simulation of ion front-ends is under development and will be used to support FRIB commissioning/operations

- Built around open source Warp family of PIC code tools
- Formulated for ease maintenance/extension with multi-users and many ion and lattice cases
  - » Allow collaborative work while extending for many cases of in ion front ends
  - » Wide range of model levels possible

Challenges significant: much physics unclear and lab diagnostics limited

- Beam emerging from ECR ion sources complex and poorly understood
- Electron neutralization models need improvement: Wong PhD project
  - » May require full 3D or thick slice 2D making much more costly models

But insight gained from code diagnostics can still help: Examples

- 3D dipole bend: placement of slanted pole magnet + space-charge compensations
- Space charge effects surprisingly benign on most ions analyzed to date
- Canonical angular momentum will impact optimization of species collimation
- ….

Much more to do: Real tests coming soon with application to FRIB data from early lab commissioning of front-end

Extra Slides

FRIB Commissioning Plan

- Two key performance parameters (KPP) at target in 2020-2021:

  1) ^{36}Ar beam with energy ≥ 200 MeV/u and current ≥ 20 pnA

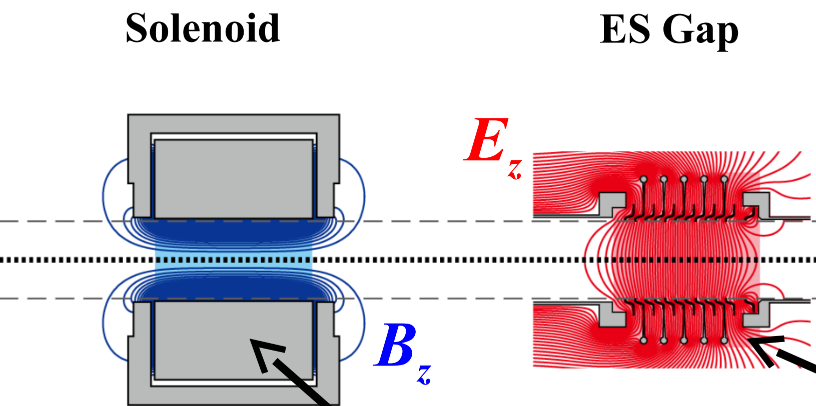
  2) ^{86}Kr beam produces ^{84}Se by fragmentation

- Single charge state and low beam power can meet KPP
- User experiments begin immediately afterwards, which requires other species and higher power (planned: 10kW in Year One)
- Acceleration of multiple charge states comes in two steps: firstly only after stripper, later starting from ion source
- Front-end commissioning begins Oct 2016 (RFQ, in 2017) with

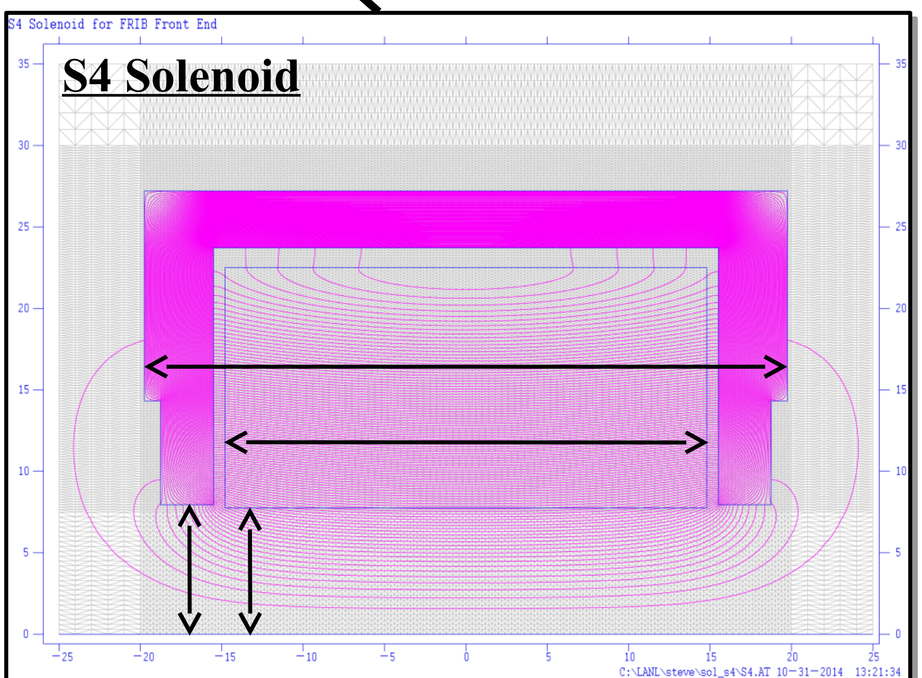
  $^{36}Ar^{18+}$ $^{86}Kr^{17+}$

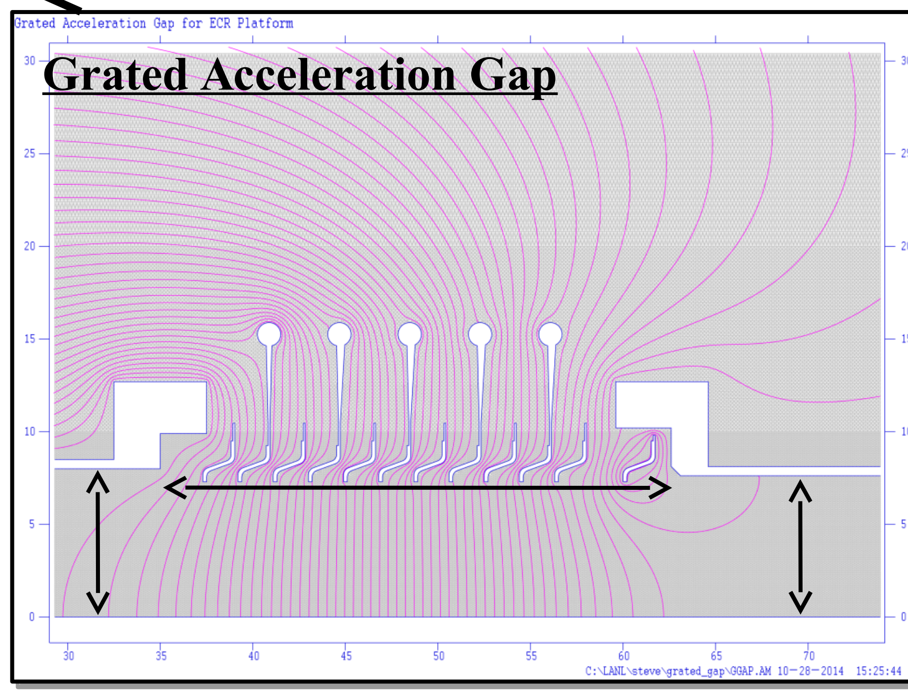
  - Normal conducting Artemis ECR ion source to start
  - Superconducting Venus ECR ion source in 2019

Solenoids and Grated Gap modeled in r-z at high resolution with Poisson



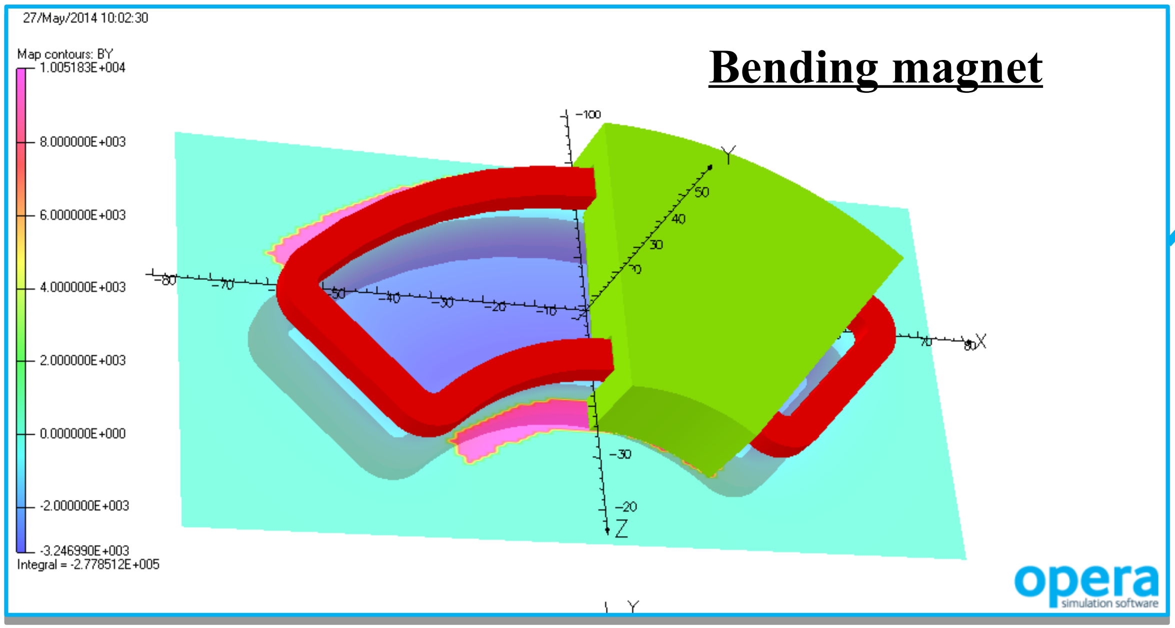
Component (Uranium)	Length [cm]	Aperture *r* [cm]
Solenoid (~0.6 Tesla)	29.6 39.52	7.75 (coil) 8.00 (magnet)
ES Gap (50 kV)	27.6	9.921 (upstream) 7.620 (downstream)

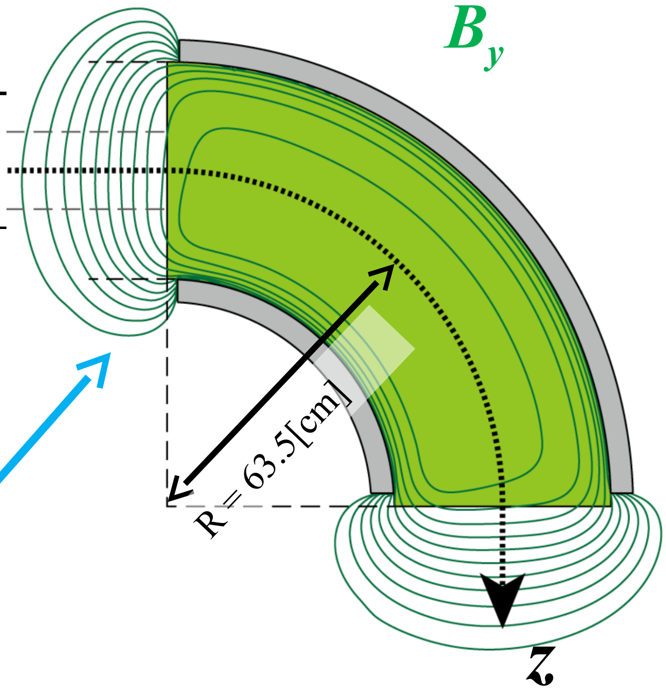




Dipole bending magnet modeled with opera in 3D

Component (Uranium)	Radial curvature [cm]	Length [cm]	Aperture [cm]
Bend (0.17 [T])	63.5	99.7456(core)	x = 20.5 y = 5.0



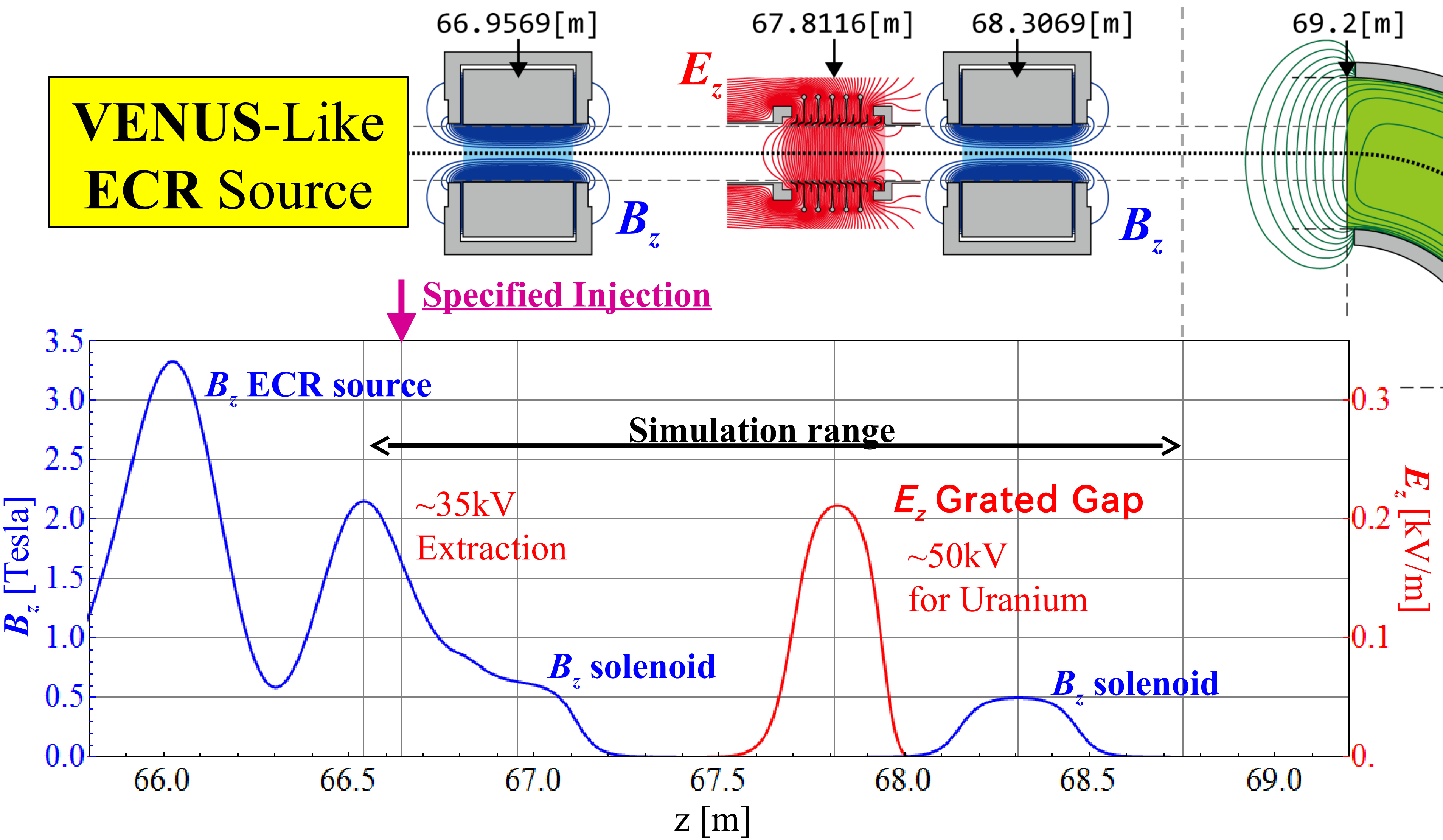


Opera (electromagnetic design) software

Ref. X. Wu, Frontend Magnets D5 & S4, 5-27-2014

Dipole has slanted poles with significant nonlinearity and extended fringe fields

Lattice Fields up to 1st Dipole

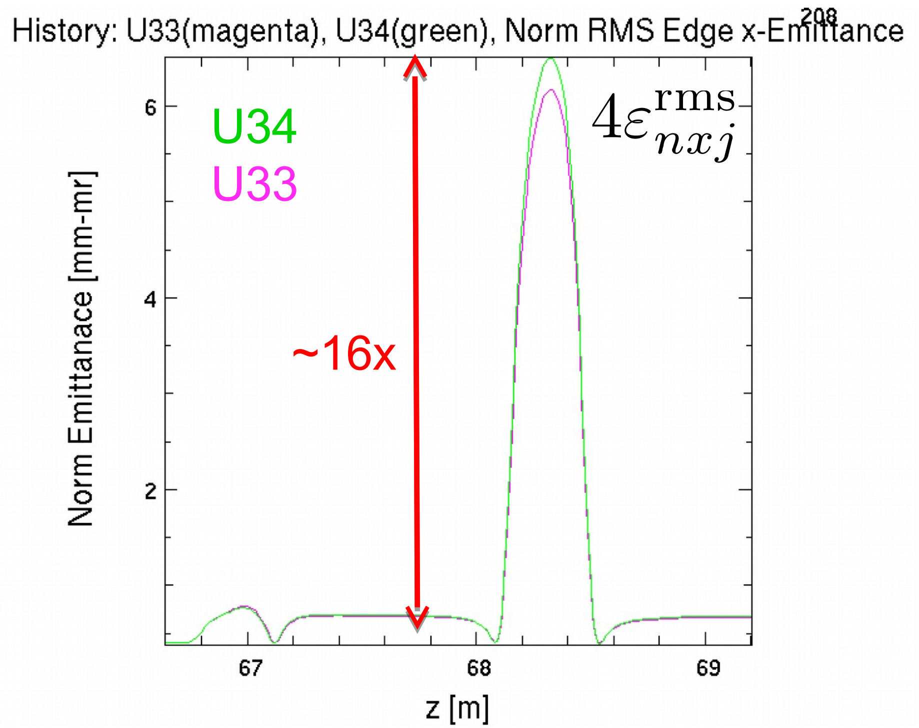


Radial normalized emittance derived in envelope model allows sensitive probing of phase-space area evolution

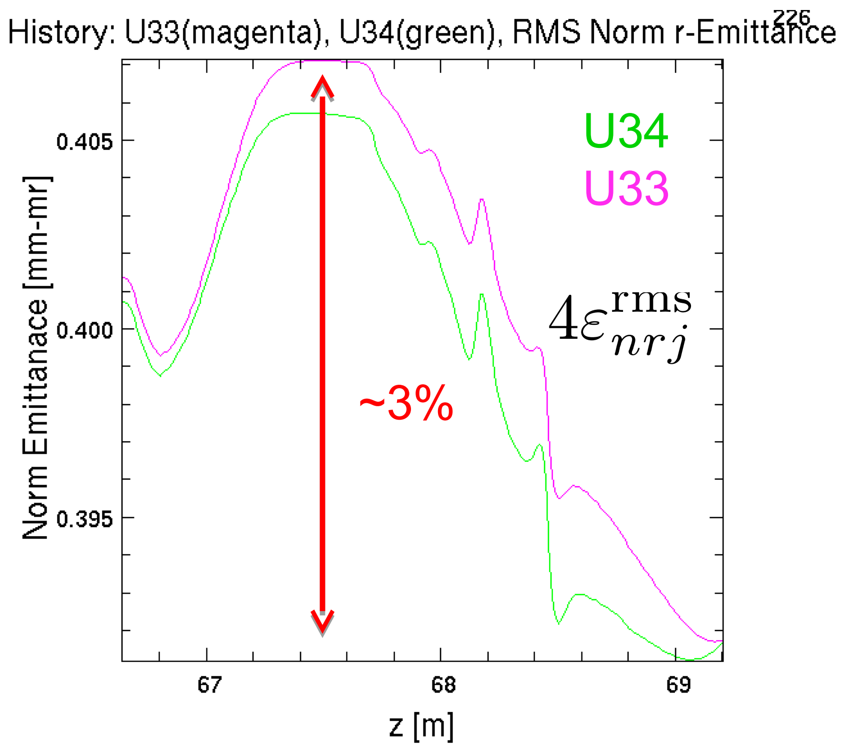
- Very little growth in radial emittance with/without applied field nonlinearities provided radial envelope evolution relatively compact

(Nonlinear Applied Fields Included)

Ordinary Normalized Emittance



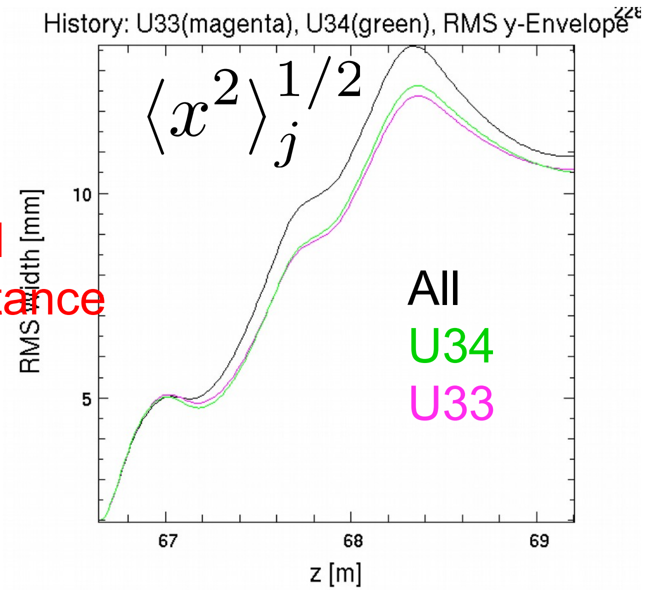
Normalized Radial Emittance



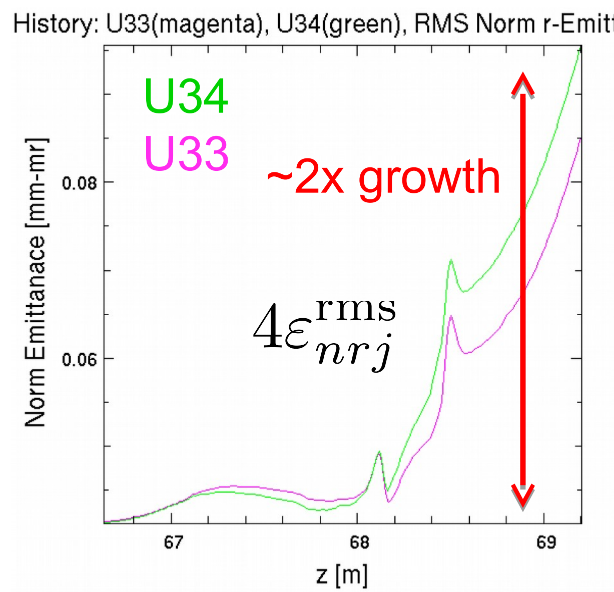
Warp simulations illustrate even when initial ions cold and emittance grows the envelope changes little due to large canonical angular mom

Low Initial
mal Emittance

rms Envelope



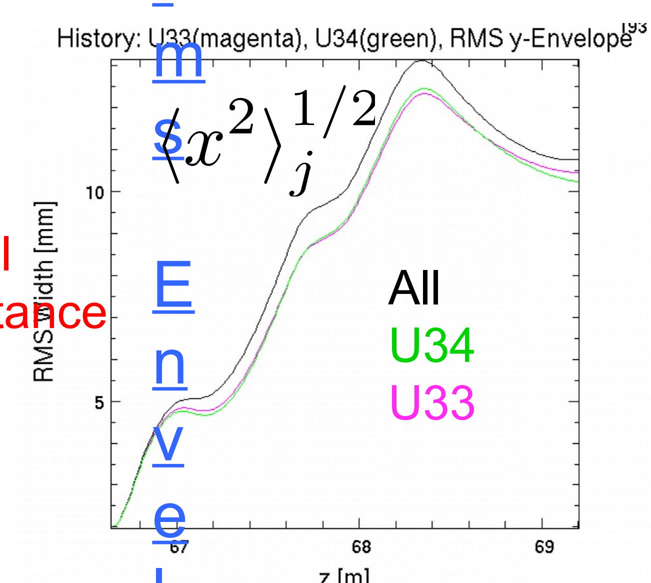
Normalized Radial Emittance



But final
value still
low!

High Initial
mal Emittance

rms Envel



Normalized Radial Emittance