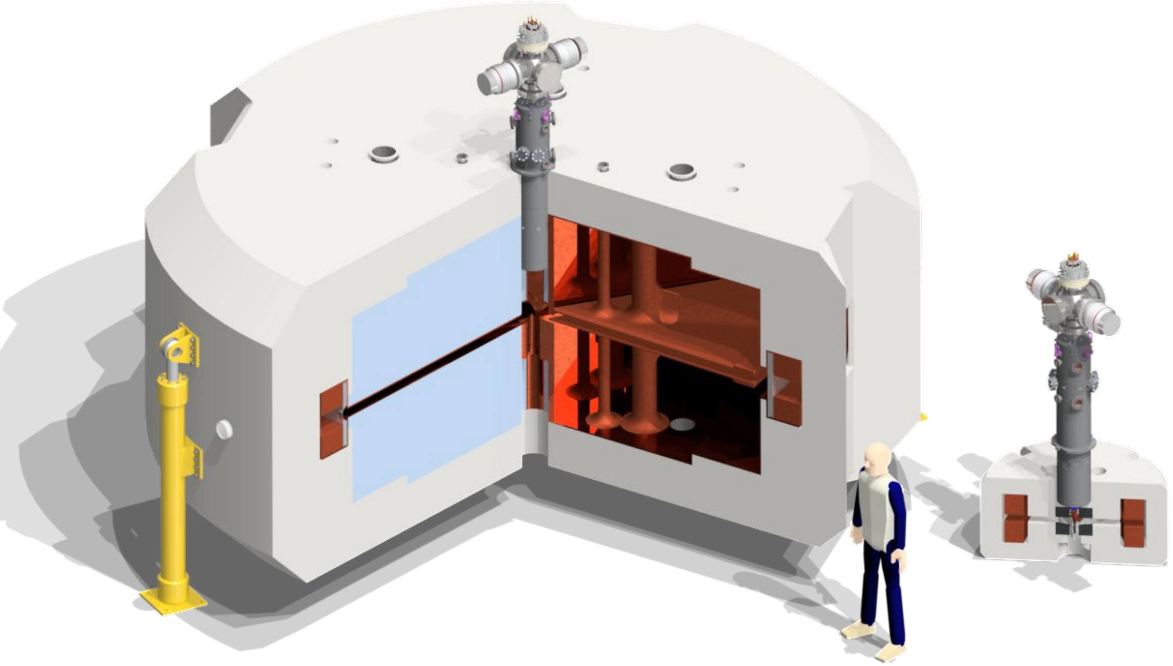
High-Fidelity Simulations and Machine Learning for Accelerator Design and Optimization

Andreas Adelmann,
Daniel Winklehner
for the IsoDAR and OPAL collaborations

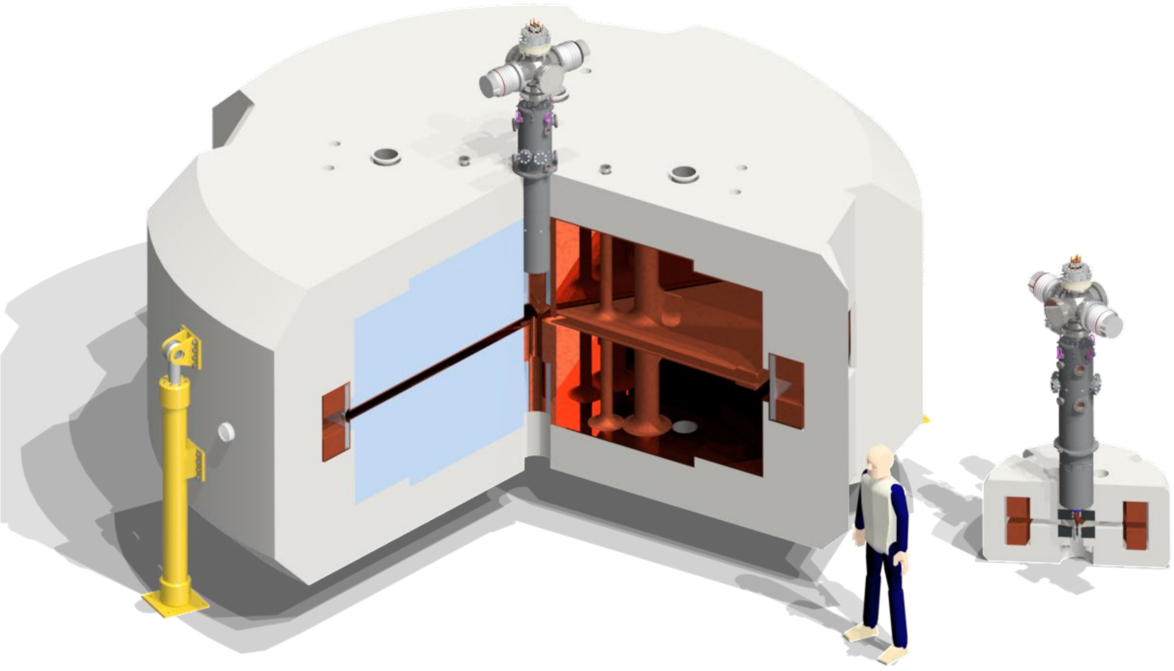
NAPAC’22 - 08/09/2022



PAUL SCHERRER INSTITUT

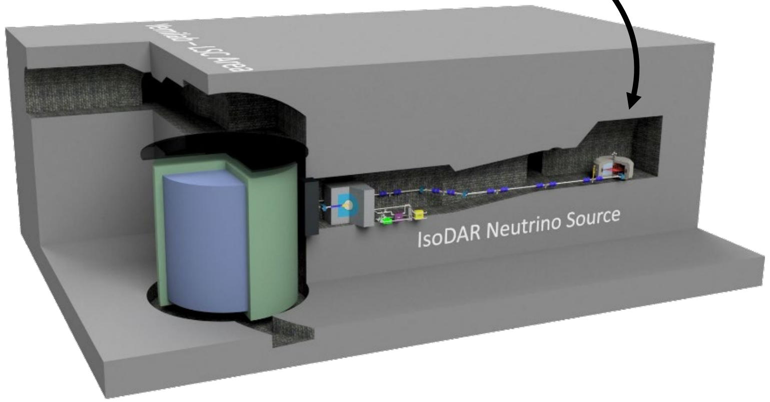
Outline

- Motivation – IsoDAR
  - The need for high-fidelity simulations
- Introduction to OPAL
- Simulation Results
- ML for Uncertainty Quantification
- ML for speeding up Optimization
- Outlook – Prototype testing
  - ML for commissioning assistance

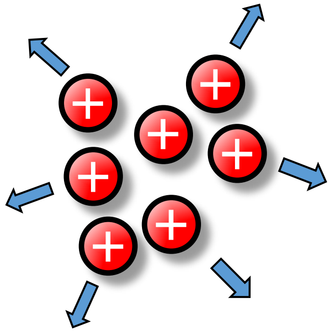


For the discovery-level experiment IsoDAR, we have specific accelerator requirements/challenges

Needs to fit here

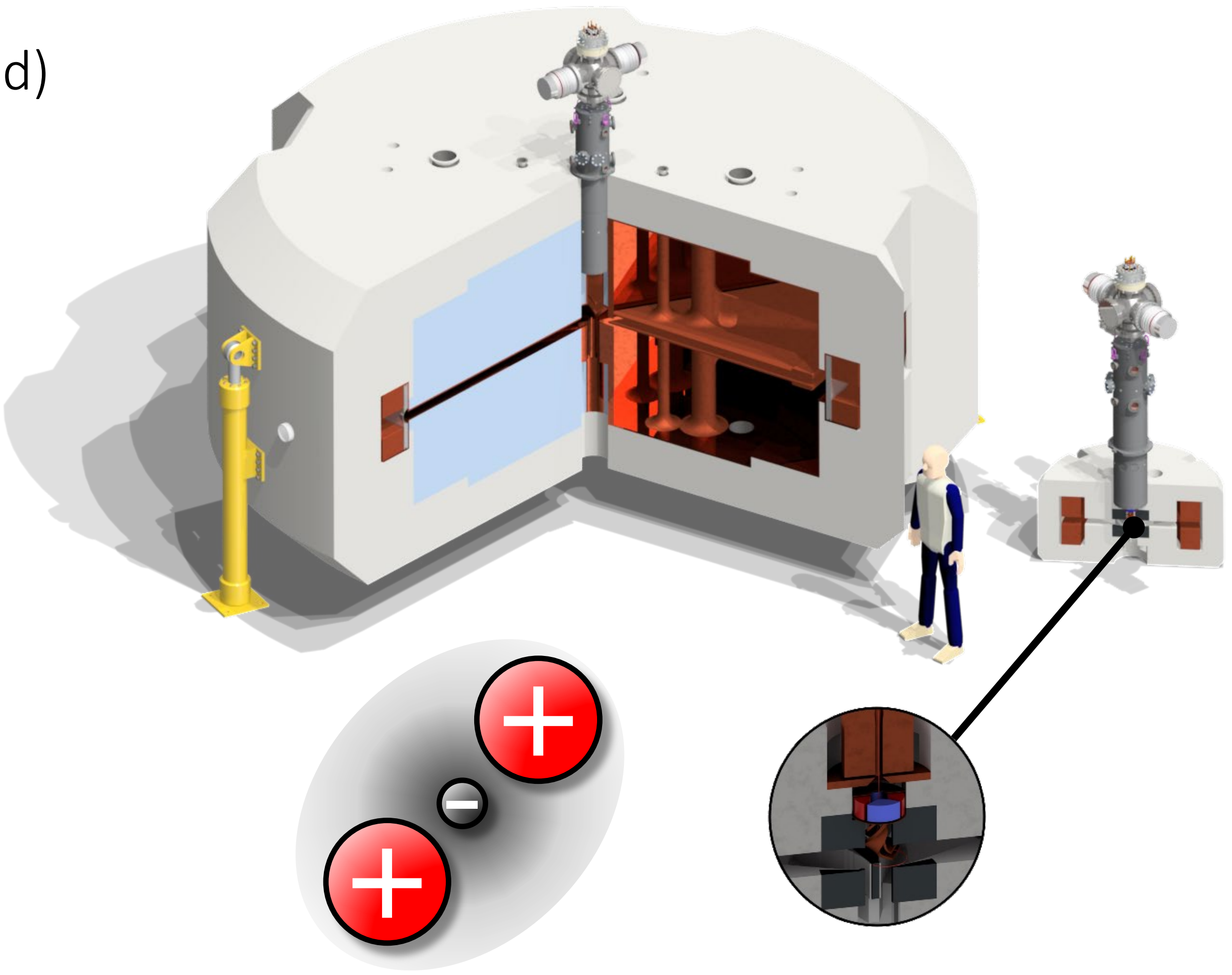


- Isotope Decay-At-Rest (IsoDAR):
  - A proposed search for additional neutrinos with world-leading sensitivity.
- Accelerator Requirements:
  - Compact, robust, cost-effective (underground installation)
  - Continuous Wave (CW) operation, 80% duty factor (for maintenance)
  - 10 mA, 60 MeV protons on target
- Challenges:
  - Related to space-charge (Coulomb-repulsion of particles in bunch)
  - Leads to beam spread and non-linear behavior
  - Beam losses which lead to activation of the machine (limit is 200 W in extraction region – PSI experience)



The HCHC-XX cyclotron design addresses these challenges

- Room-temperature coils (no cryogenics needed)
- Isochronous, cw, 80% duty factor
- Operates at 32.8 MHz (4th harmonic)
- 4 double-gap cavities
  → high energy gain/turn
- Accelerates H_2^+ ions instead of protons
- Direct axial injection through a Radiofrequency Quadrupole (RFQ)
  - Efficient bunching
  - Moderate pre-acceleration
- Utilizes vortex motion
  (a beam dynamics effect during acceleration)

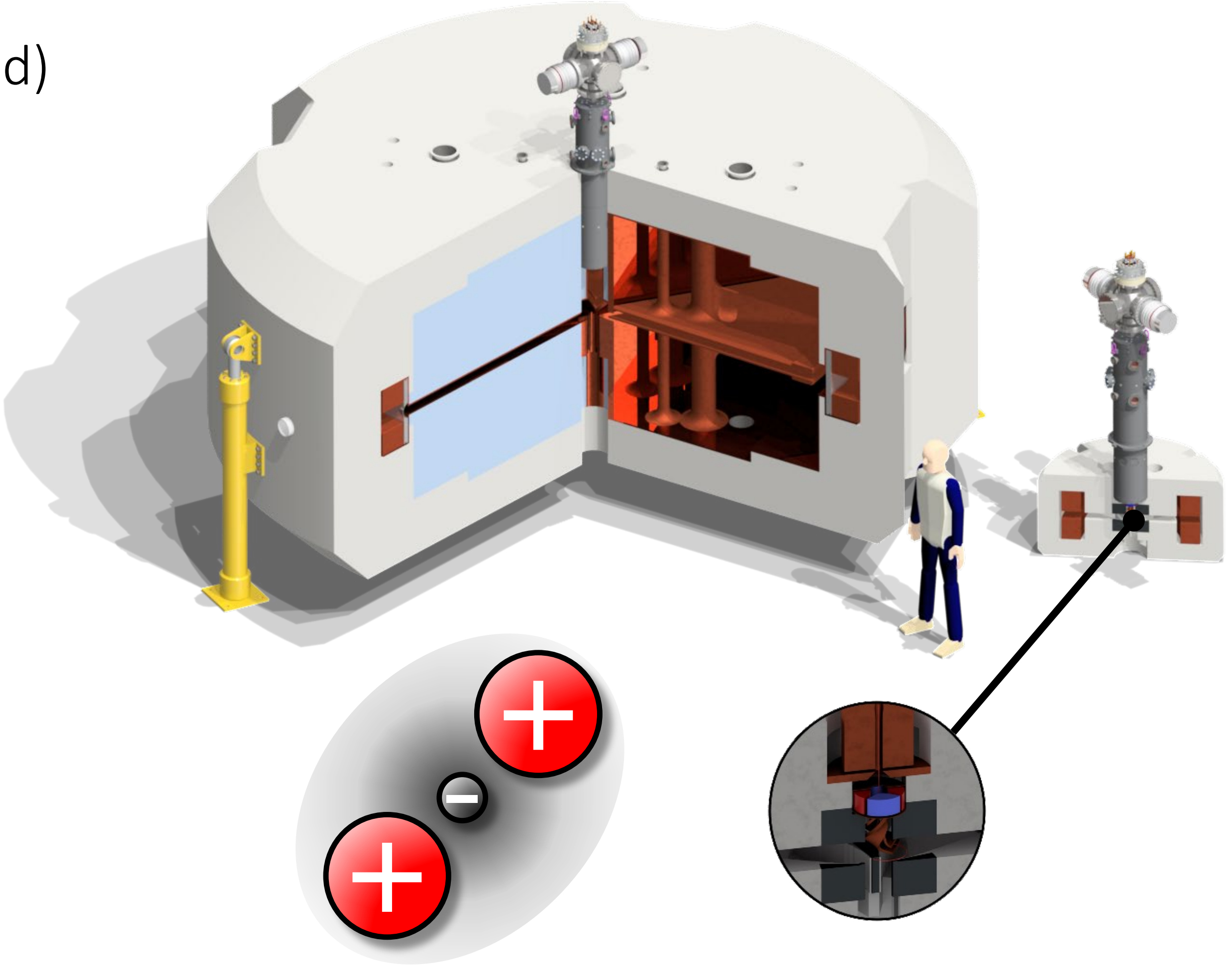


The HCHC-XX cyclotron design addresses these challenges

- Room-temperature coils (no cryogenics needed)
- Isochronous, cw, 80% duty factor
- Operates at 32.8 MHz (4th harmonic)
- 4 double-gap cavities
  → high energy gain/turn
- Accelerates H_2^+ ions instead of protons

Need for Hi-Fi Simulation

- Direct axial injection through a Radiofrequency Quadrupole (RFQ)
  - Efficient bunching
  - Moderate pre-acceleration
- Utilizes vortex motion
  (a beam dynamics effect during acceleration)
- < 200 W losses = O(1e-4) relative loss
  → O(1e6) particles needed to resolve in sim



To accurately simulate the sensitive and complicated effects in the cyclotron, we use the Particle-In-Cell (PIC) code OPAL

A. Adelmann, A. Albà (PSI), P. Calvo (CIEMAT),
M. Frey (U. St Andrews), A. Gsell (PSI), Ch. Kraus,
S. Muralikrishnan (PSI), Ch. Rogers (RAL), J. Snuverink (PSI),
N. Neveu (SLAC), D. Winklehner (MIT)

PAUL SCHERRER INSTITUT PSI · MIT · Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas · University of St Andrews · UKRI Science and Technology Facilities Council ISIS Neutron and Muon Source · SLAC NATIONAL ACCELERATOR LABORATORY

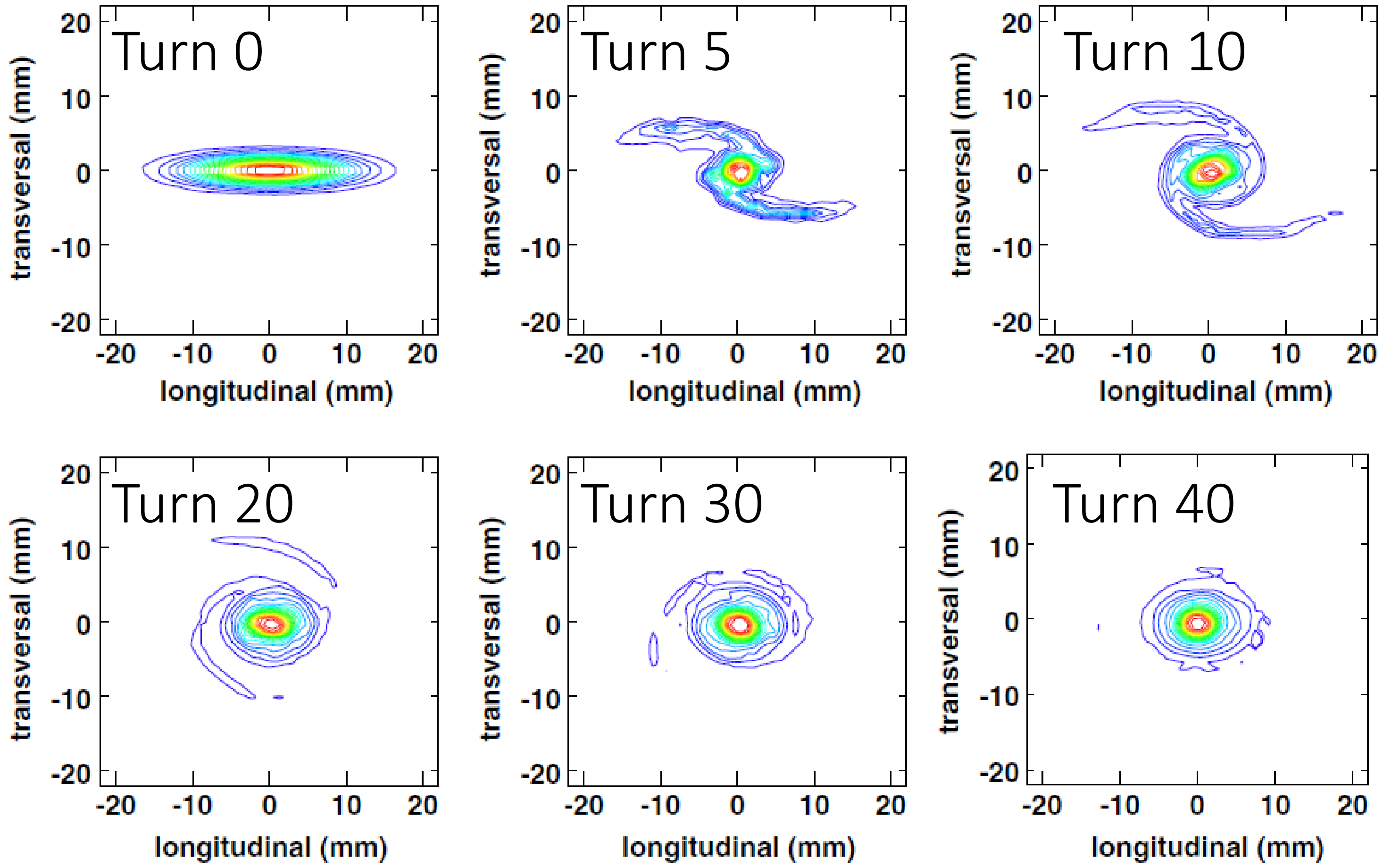
Object Oriented Parallel Particle Library (OPAL)

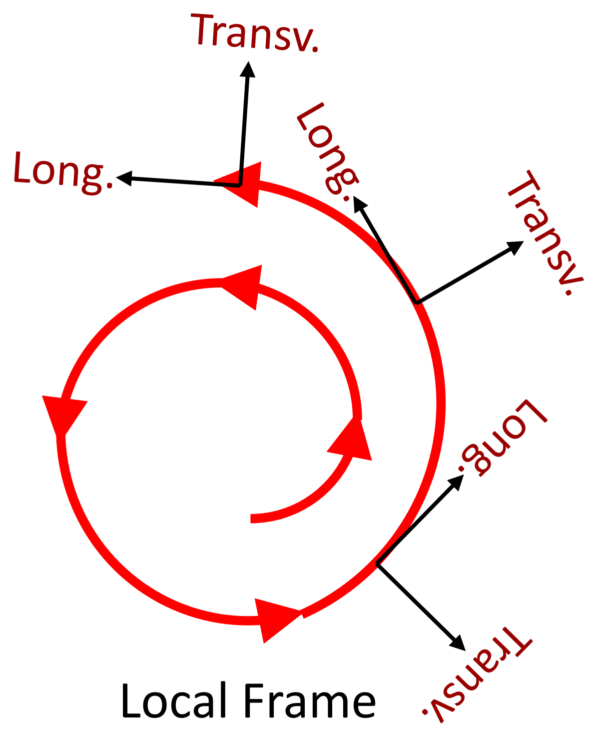
https://gitlab.psi.ch/OPAL/src/wikis/home

OPAL is a versatile open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D EM field calculation, collisions, radiation, particle-matter interaction, and multi-objective optimisation

- OPAL is built from the ground up as an HPC application
- OPAL runs on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions
- OPAL is written in C++, uses design patterns, easy to extend
- The OPAL Discussion Forum:
  https://psilists.ethz.ch/sympa/info/opal
- International team of 11 active developers and a user base of $\mathcal{O}(100)$
- The OPAL **sampler** command can generate labeled data sets using the largest computing resources and allocations available

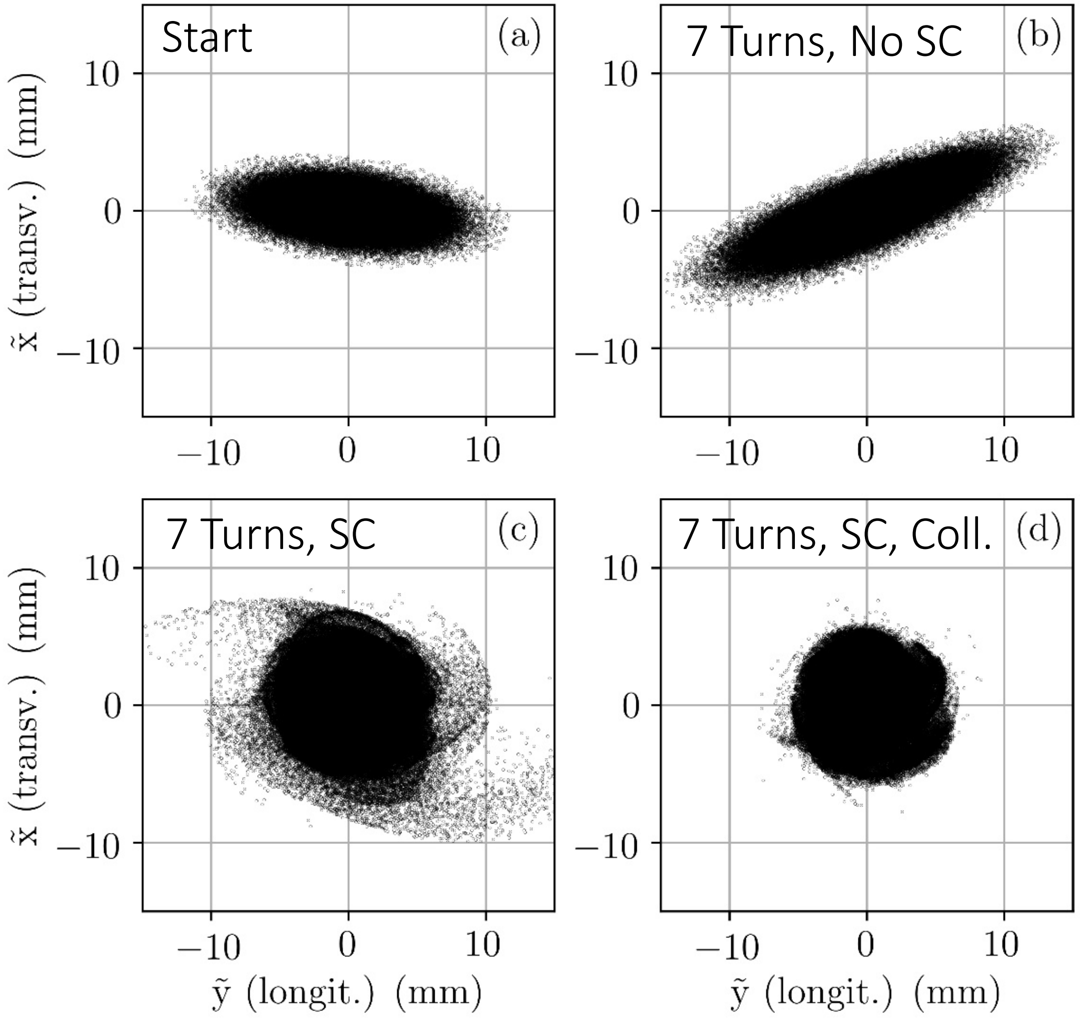
Vortex motion – Discovered in PSI Injector II Simulated with OPAL → Good Agreement





Yang et al. **PRSTAB** (2010) https://journals.aps.org/prab/abstract/10.1103/PhysRevSTAB.13.064201

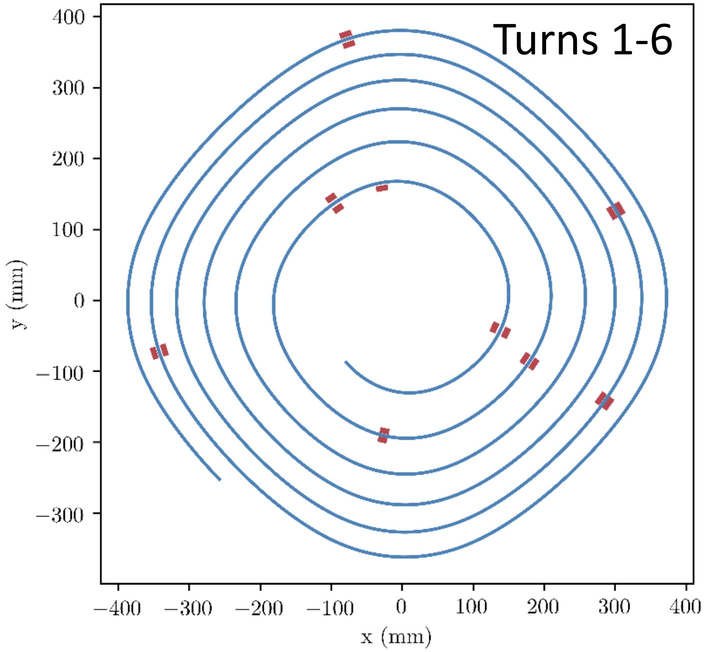
Vortex Motion in the IsoDAR 60 MeV/amu cyclotron simulated with OPAL

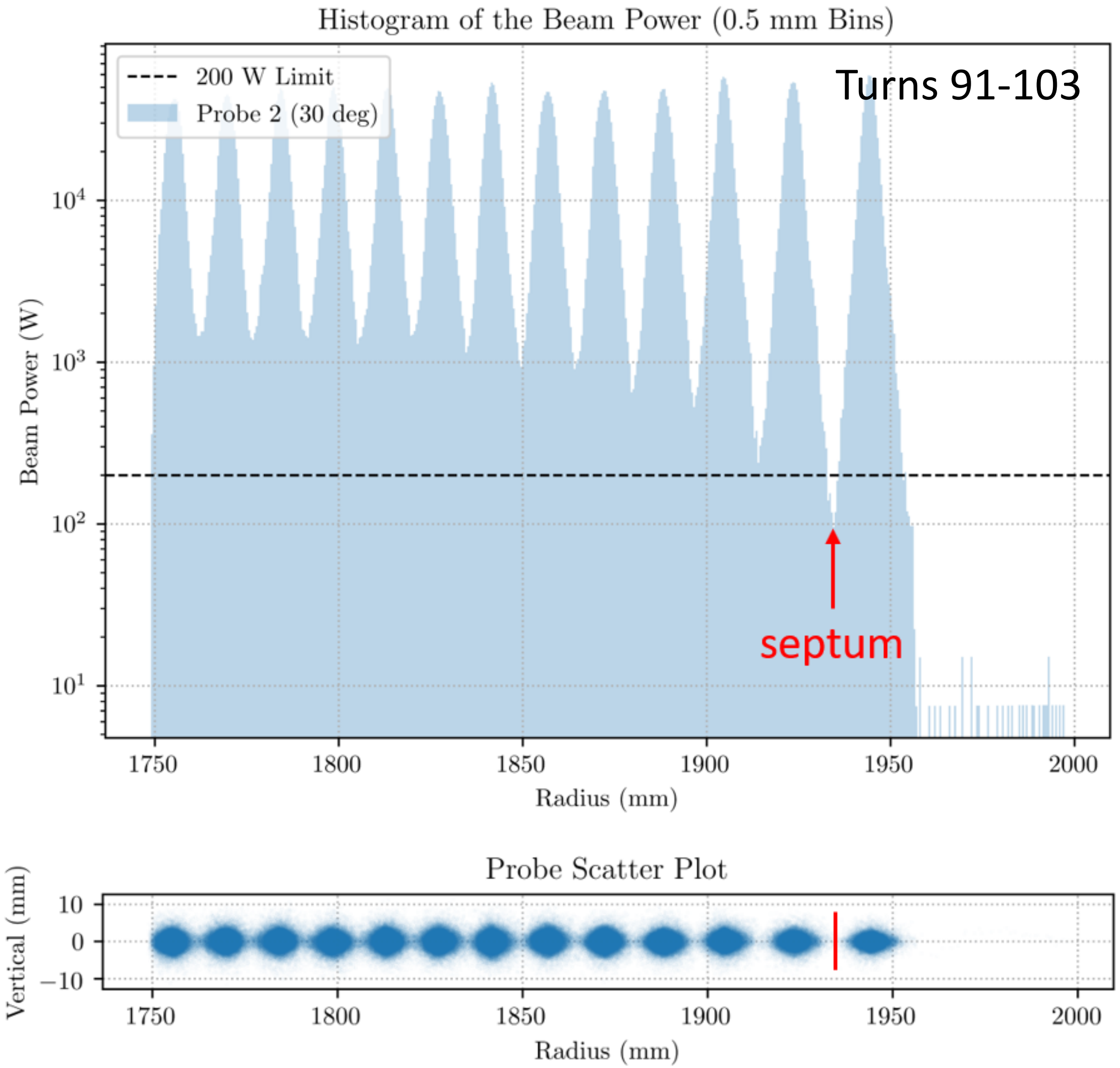


DW et al., **New J. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001

Optimize phase, RF voltage, cavity shape, collimator placement

- Phase: -5°, V = 70-240kV
- Collimate Halo → ~30% loss
- 98 W on septum (~1e-4 rel.)

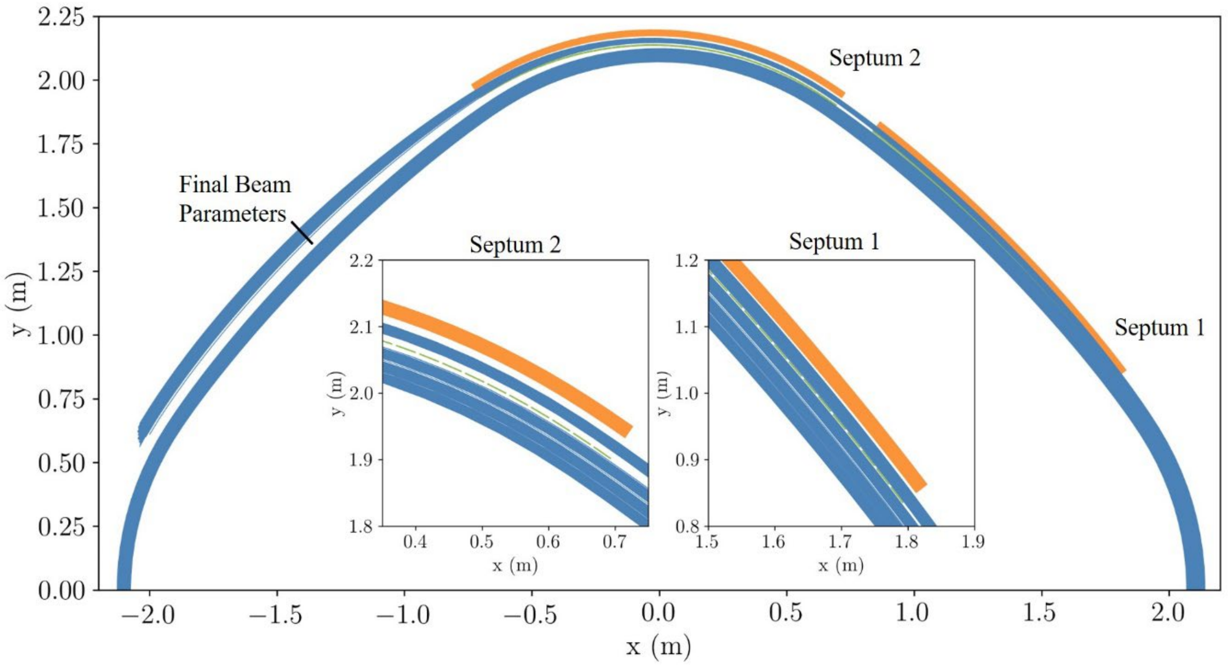




DW et al., **New J. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001

Beam can be extracted with good quality

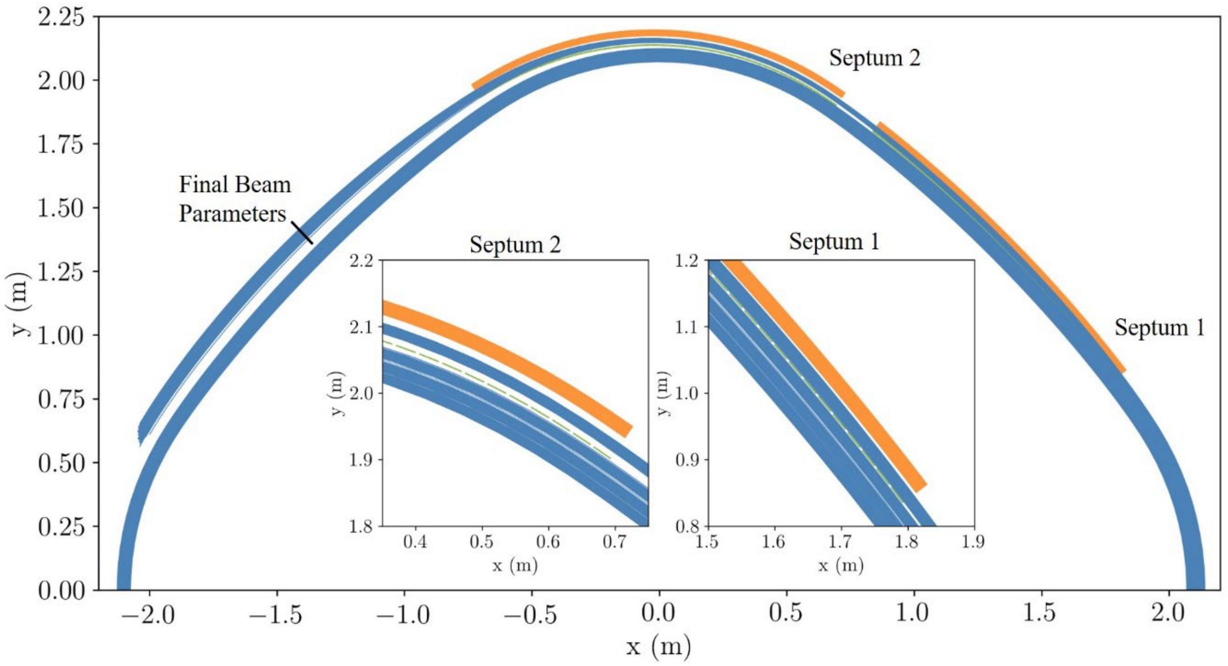
- Minimal losses at 60 MeV/amu: < 100 Watt (factor 2 below 200 W limit)!
- RMS Size:
  - Radial: 7.5 mm
  - Longitudinal: 11 mm
  - Vertical: 1.9 mm
- RMS, normalized emittance:
  - vertical: 0.44 mm-mrad
  - Radial: 3.8 mm-mrad
- Longitudinal emittance:
  - 0.1 MeV-deg



DW et al., **New J. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001

Beam can be extracted with good quality

- Minimal losses at 60 MeV/amu: < 100 Watt (factor 2 below 200 W limit)!
- RMS Size:
  - Radial: 7.5 mm
  - Longitudinal: 11 mm
  - Vertical: 1.9 mm
- RMS, normalized emittance:
  - vertical: 0.44 mm-mrad
  - Radial: 3.8 mm-mrad
- Longitudinal emittance:
  - 0.1 MeV-deg



- Is it robust?
  Use Surrogate Modeling (AI/ML) for Uncertainty Quantification (see next slides)

DW et al., **New J. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001

Excellent opportunity to use machine learning ("Virtual Accelerators")

- Particle accelerator simulations can be complex with large sets of input parameters
- Optimization requires repeated evaluation of points in parameter-hyperspace.
- Surrogate model: train neural net on sparse set of points in this hyperspace
- Evaluation of surrogate model is orders of magnitude faster than original simulation
  - Uncertainty Quantification (using PCE)
  - Optimization
  - Real-Time Feedback

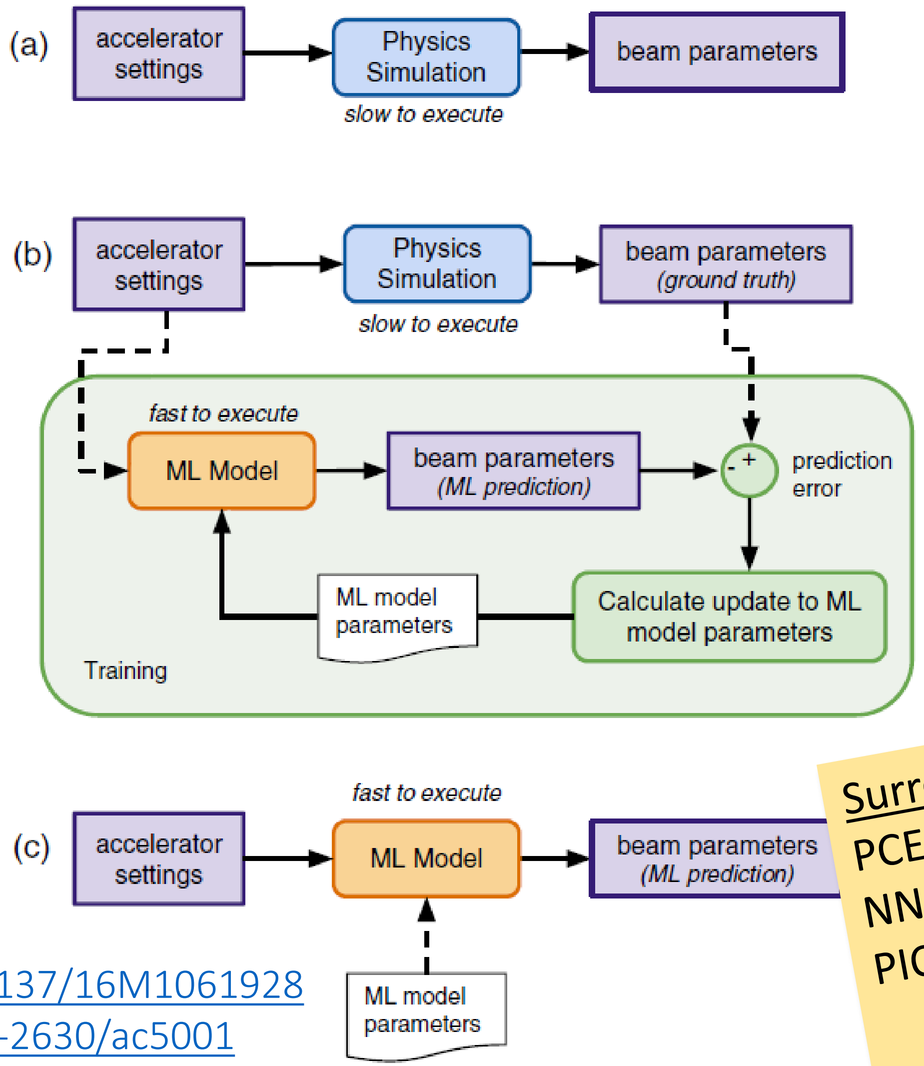


Image: A. Edelen et al. *PRAB* 23, 044601 (2020)

<u>Surrogate Model</u>
PCE or a ML-trained NN to replace costly PIC simulations.

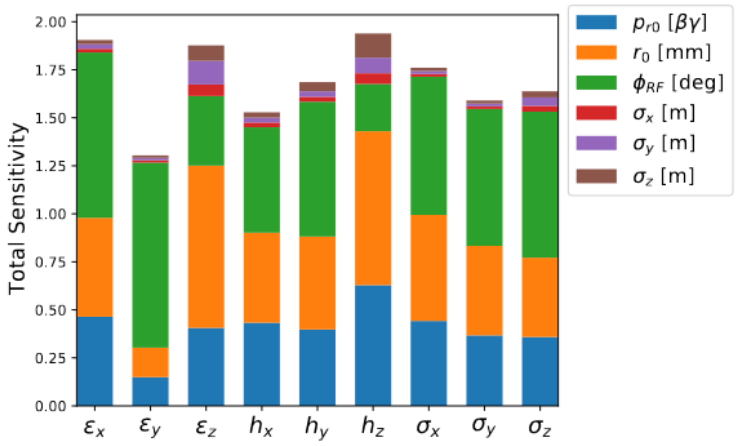
AA **SIAM/ASA J. Uncert. Quant.** (2019) https://epubs.siam.org/doi/10.1137/16M1061928
D. Winklehner et al., **New J. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001
D. Koser et al. **Front. Phys.** (2022) https://arxiv.org/abs/2112.02579

Uncertainty Quantification using Polynomial Chaos Expansion (PCE)-based SM shows robust cyclotron design

- Surrogate model using Polynomial Chaos Expansion (PCE)
- Input parameters:

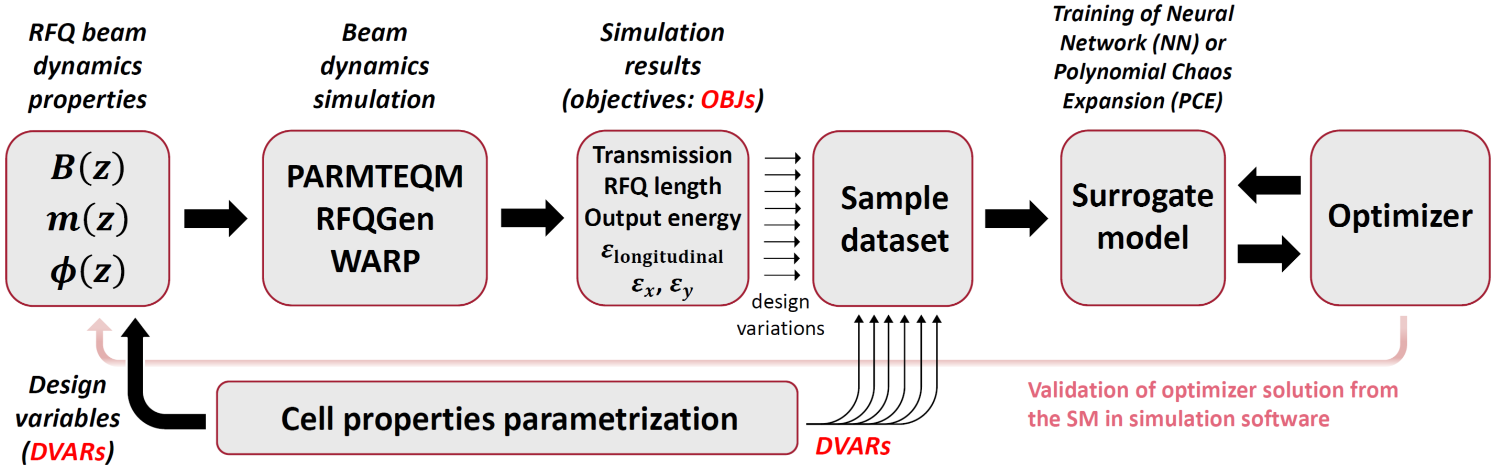
	p_{r0} $[\beta\gamma]$	r_0 [mm]	ϕ_{rf} [deg]	σ_x [m]	σ_y [m]	σ_z [m]
Lower	0.00225	115.9	283.0	0.00095	0.00285	0.00475
Upper	0.00235	119.9	287.0	0.00105	0.00315	0.00525

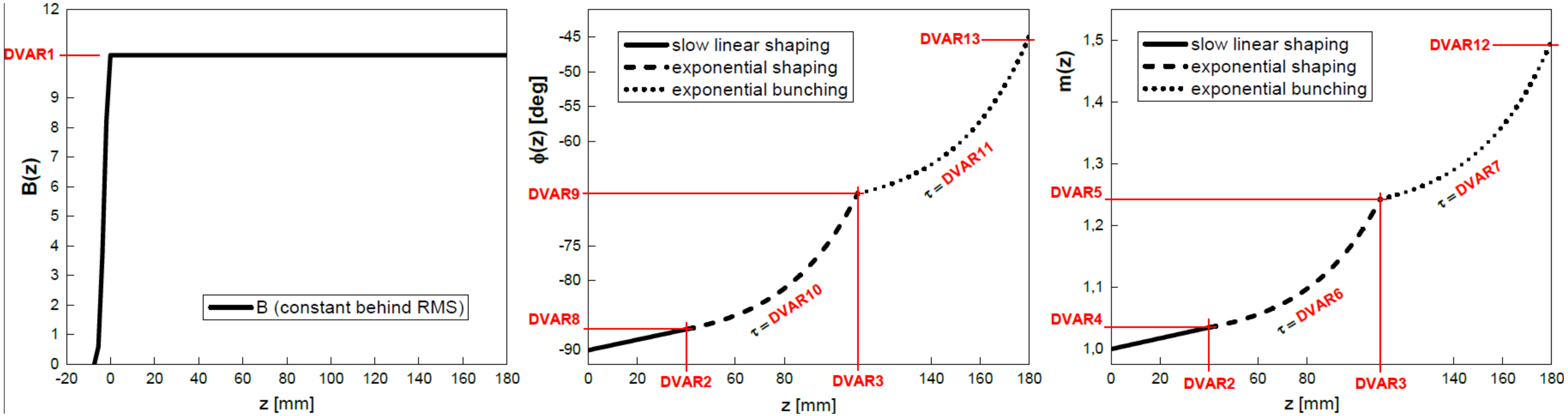
- Quantities of Interest (QoI): Beam size, Halo parameter, Emittance
- Yields Sobol' indices indicate sensitivity of system to variation of certain input parameters
- Robust vs. beam size changes
- Other parameters are slow-changing or can be quickly adjusted in a feedback system ✓



- Also for collimator placement to determine optimal design ✓

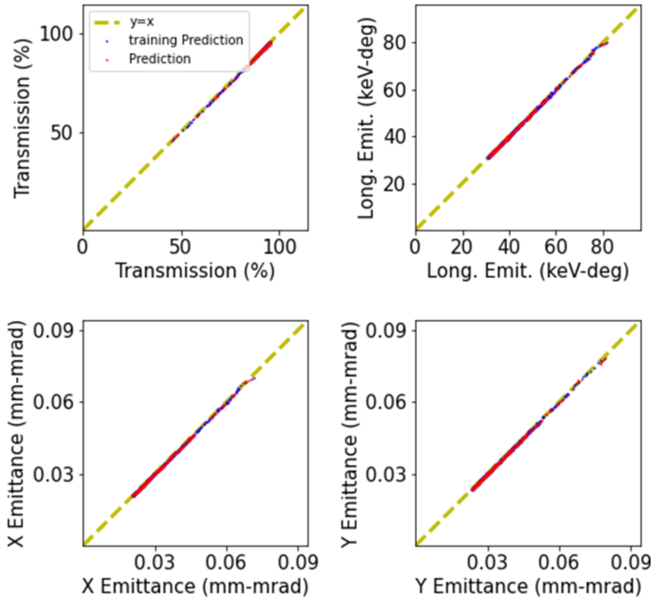
RFQ Parametrization – Surrogate Modelling - Optimization



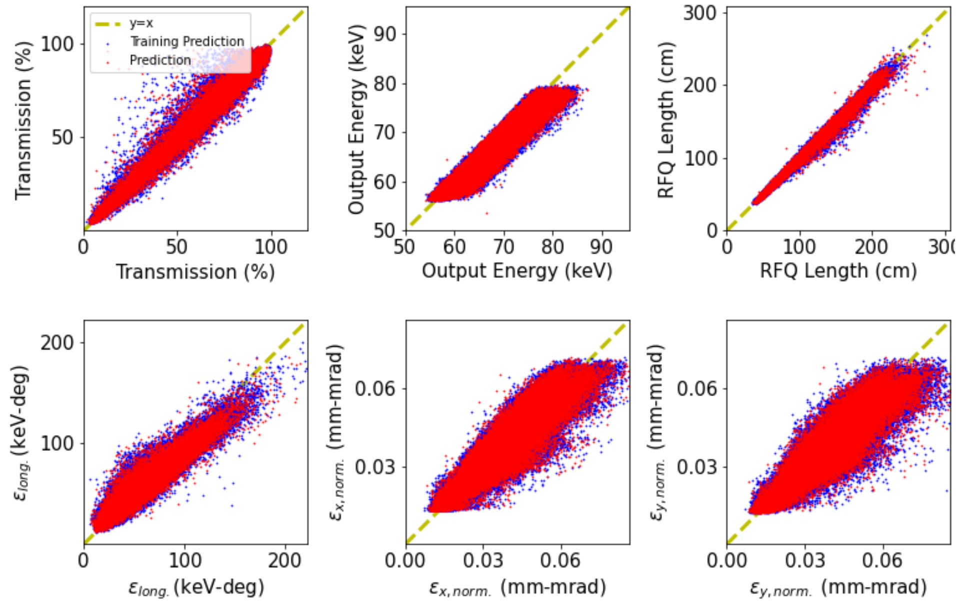


Koser et al. **Front. Phys.** (2022) https://arxiv.org/abs/2112.02579

- Excellent results for Twiss parameters
- Bodes well for tuning assistant

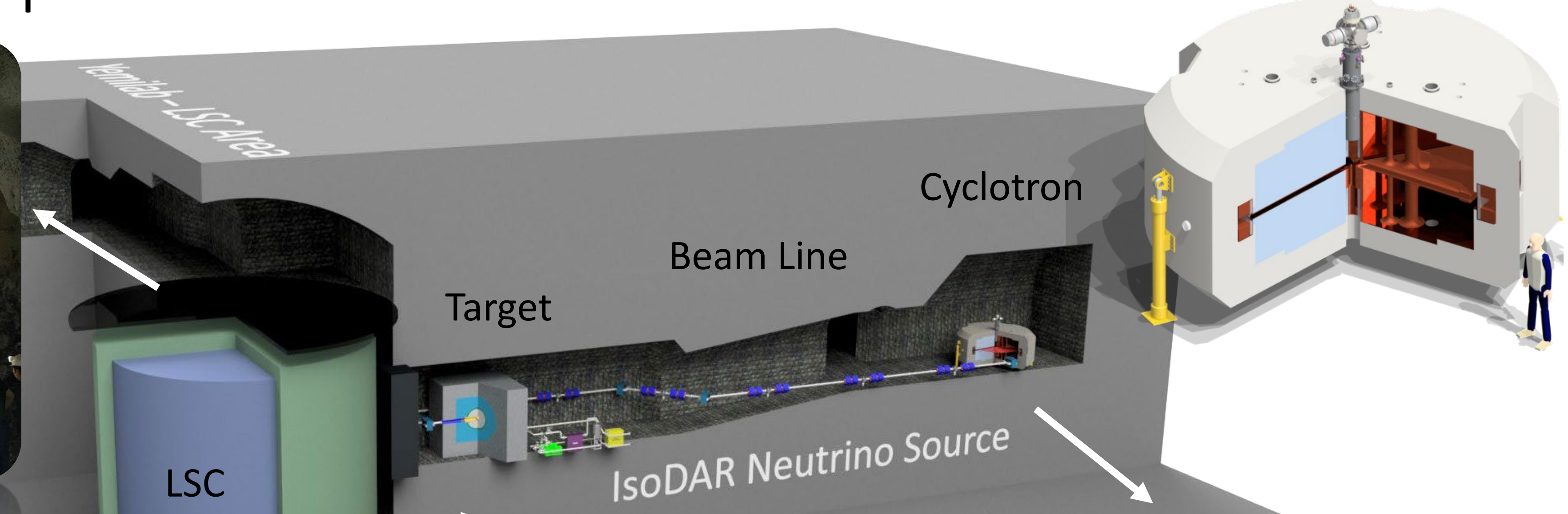


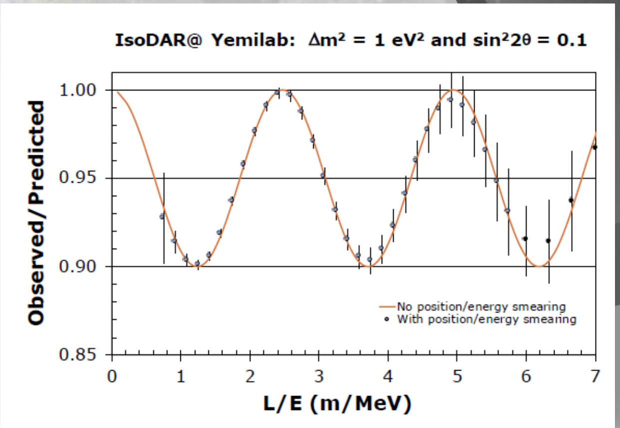
- Challenges with RFQ mechanical design prediction
- Interesting avenue of research!
- Can already be used to restrict parameter space for optimization



Koser et al. **Front. Phys.** (2022) https://arxiv.org/abs/2112.02579

With robust, optimized design, IsoDAR is pre-approved to run at Yemilab in Korea





Caverns are already constructed

Physics Paper: http://arxiv.org/abs/2111.09480, PRD 2022
IsoDAR@Yemilab – CDR: http://arxiv.org/abs/2110.10635 arXiv 2021

Thank You!

NSF

IsoDAR: International collaboration of ~30 scientists

MIT

UNIVERSITY OF MICHIGAN

COLUMBIA UNIVERSITY IN THE CITY OF NEW YORK

University of HUDDERSFIELD

INFN

Institute for Basic Science ibs 기초과학연구원

PAUL SCHERRER INSTITUT PSI

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

Industry Partners

AIMA DEVELOPPEMENT

Best® Cyclotron Systems

BEVATECH

iba

BARTOSZEK ENGINEERING

References

- IsoDAR@Yemilab – CDR: IsoDAR Collaboration **arXiv** (2021) arxiv:2110.10635
- IsoDAR@Yemilab – Physics: J. Spitz, … DW, … **PRD** (2022) arxiv:2111.09480
- Ion Source: D. Winklehner et al. **RSI** (2021) https://arxiv.org/abs/2008.12292
- RFQ-DIP: D. Winklehner et al. **RSI** (2016) https://aip.scitation.org/doi/abs/10.1063/1.4935753
- RFQ-DIP: D. Winklehner et al. **NIMA** (2018) https://arxiv.org/abs/1807.03759
- Uncertainty Quantification: A. Adelmann **SIAM/ASA J. Uncert. Quant.** (2019) https://epubs.siam.org/doi/10.1137/16M1061928
- ML for RFQ: D. Koser et al. **Front. Phys.** (2022) https://arxiv.org/abs/2112.02579
- Spiral Inflector: D. Winklehner et al. **PRAB** (2017) https://arxiv.org/abs/1612.09018
- Cyclotron: D. Winklehner et al. **New Journ. Phys.** (2022) https://doi.org/10.1088/1367-2630/ac5001
- Isotopes: J. Alonso et al. **Nature** (2019) https://www.nature.com/articles/s42254-019-0095-6
- Isotopes: L. Waites et al. **EJNMMI** (2020) https://doi.org/10.1186/s41181-020-0090-3
- Target, ^{8}Li yield: A. Bungau et al. **arXiv** (2018) https://arxiv.org/abs/1805.00410
- Target, shielding: A. Bungau et al. **arXiv** (2019) https://arxiv.org/abs/1909.08009
- First experimental tests: D. Winklehner et al. **JINST** (2015) arXiv:1508.03850
- Vortex Motion: Yang et al. **PRSTAB** (2010) PhysRevSTAB.13.064201
- The OPAL Code: Adelmann et al. **arXiv** (2019) https://arxiv.org/abs/1905.06654
- High-Power Cyclotron Report: D. Winklehner et al. **arXiv** (2022) https://arxiv.org/abs/2203.07919