Office of Nuclear Physics
Exploring Nuclear Matter - Quarks to Stars

Argonne NATIONAL LABORATORY

... for a brighter future

Wish-List for Large-Scale Simulations for Future Radioactive Beam Facilities

International Computational Accelerator Physics Conference
Oct. 2-6, 2006
Chamonix, France

Jerry Nolen, Physics Division

U.S. Department of Energy

THE UNIVERSITY OF CHICAGO

Office of Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory managed by The University of Chicago

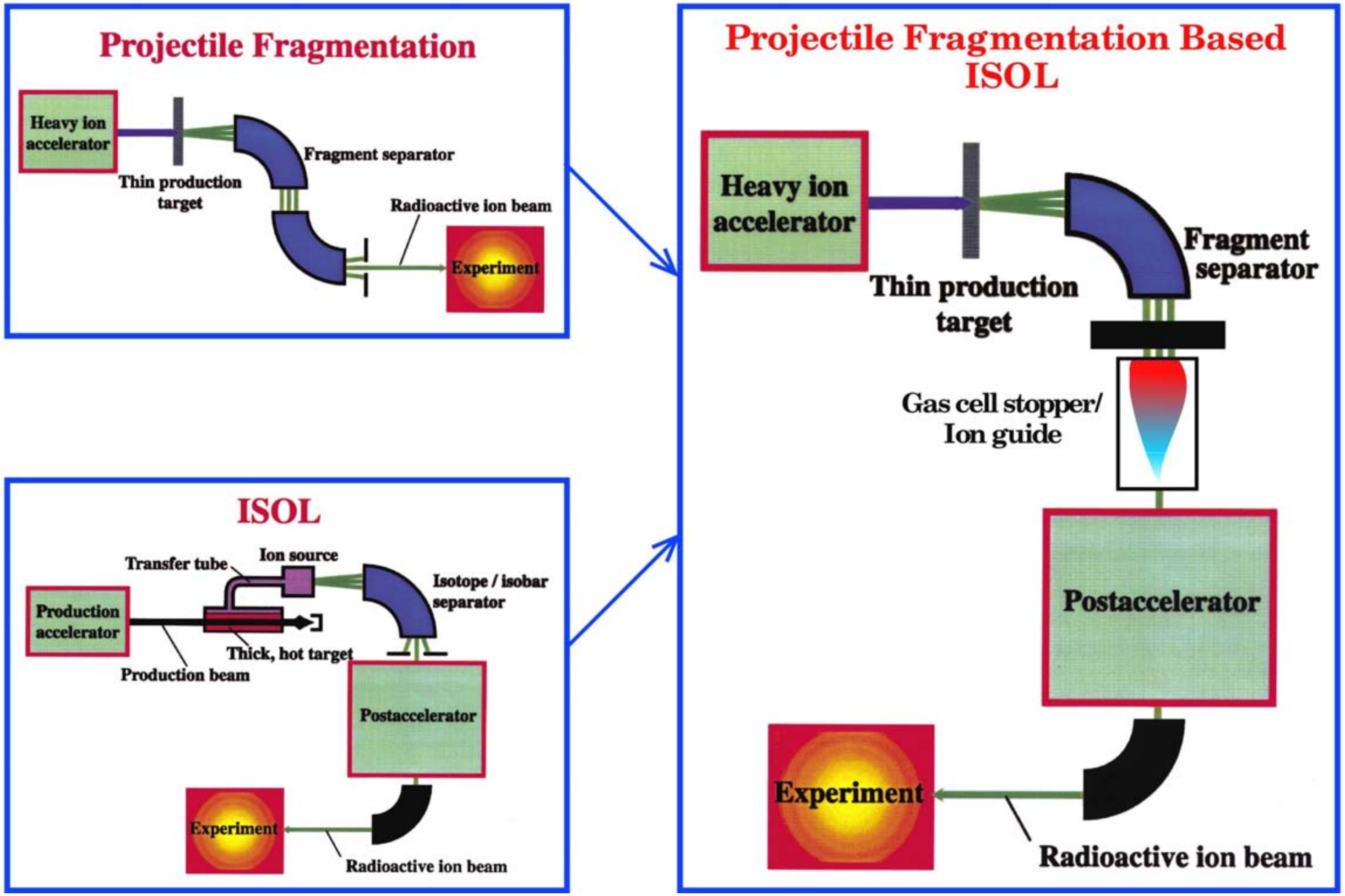
Outline

- Next generation radioactive beam facilities based on heavy-ion drivers
  - RIKEN/RI Factory in Japan (superconducting cyclotron)
  - GSI/FAIR in Germany (superconducting synchrotron)
  - RIA-lite in the U.S. (superconducting linac)
- Peta-flop computing power in the near future
- Large-scale simulation needs for design optimization
  - Complex magnet and RF cavity design
  - Detailed beam halo and loss sensitivity to alignment and parameter uncertainties
  - Detailed shielding and activation simulations
  - Fragment separator resolving power optimization coupled to radiological heating, activation, and damage minimization
- Large-scale computations applied to operation: A Model-Driven Accelerator
  - On-line peta-scale computing for near real-time tune optimization based on diagnostics feedback and detailed facility model

Rare Isotope Production Schemes

Physics drives the need for a variety of production mechanisms and rare isotope beams in 4 energy regimes

- Fast Extraction Times (~msec)
- Chemical independence
- Isobar separation



Nuclear Astrophysics with Radioactive Beams - Examples

PRL 82, 3964(1999)

PRC 65, 035803(2002)

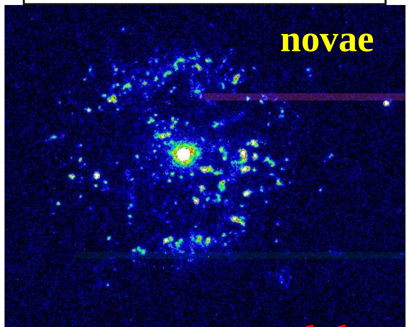
PRC 67, 065808(2003)

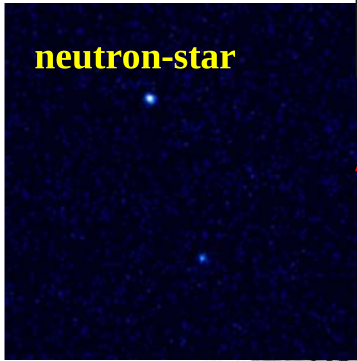
PRC 67, 065809(2003)

^{21}Na(p,α)^{18}Ne

^{15}O(α,γ)^{19}Ne

^{17}F(p,α)^{14}O





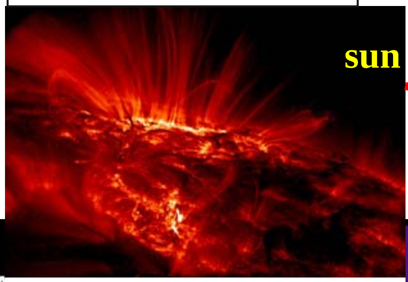
^{56}Ni(p,γ)^{57}Cu

PRL 80, 676(1998)

^{11}C(p,α)^{8}B

NPA 734, 615(2004)

^{8}B(β^+,ν) → 2α



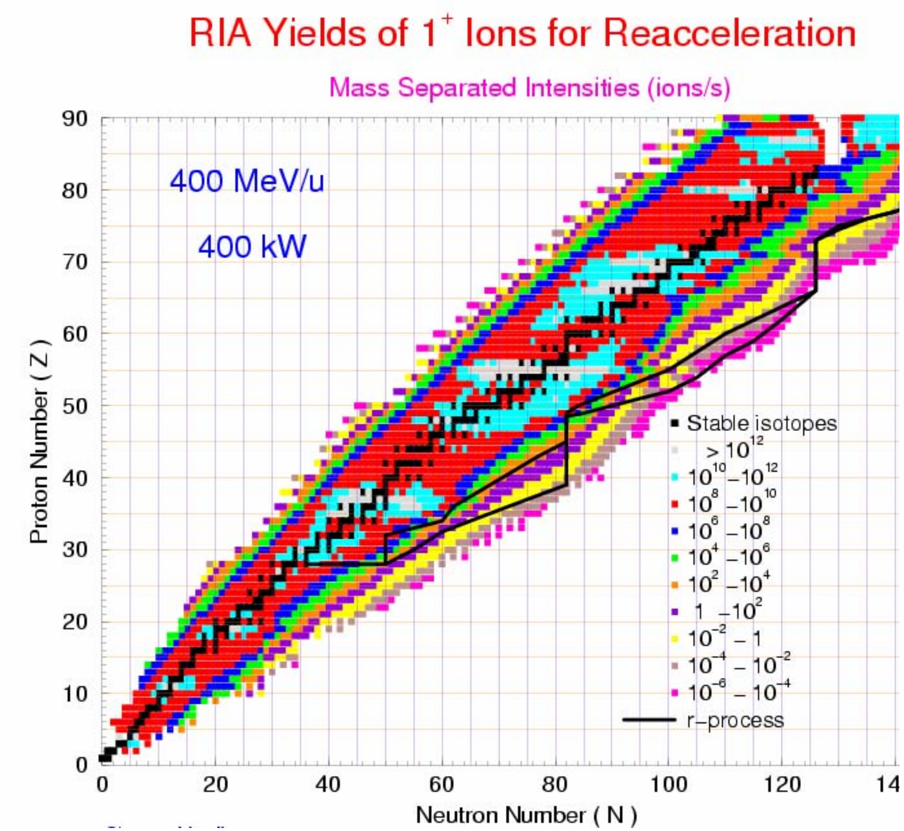
PRL 91, 252501(2003)

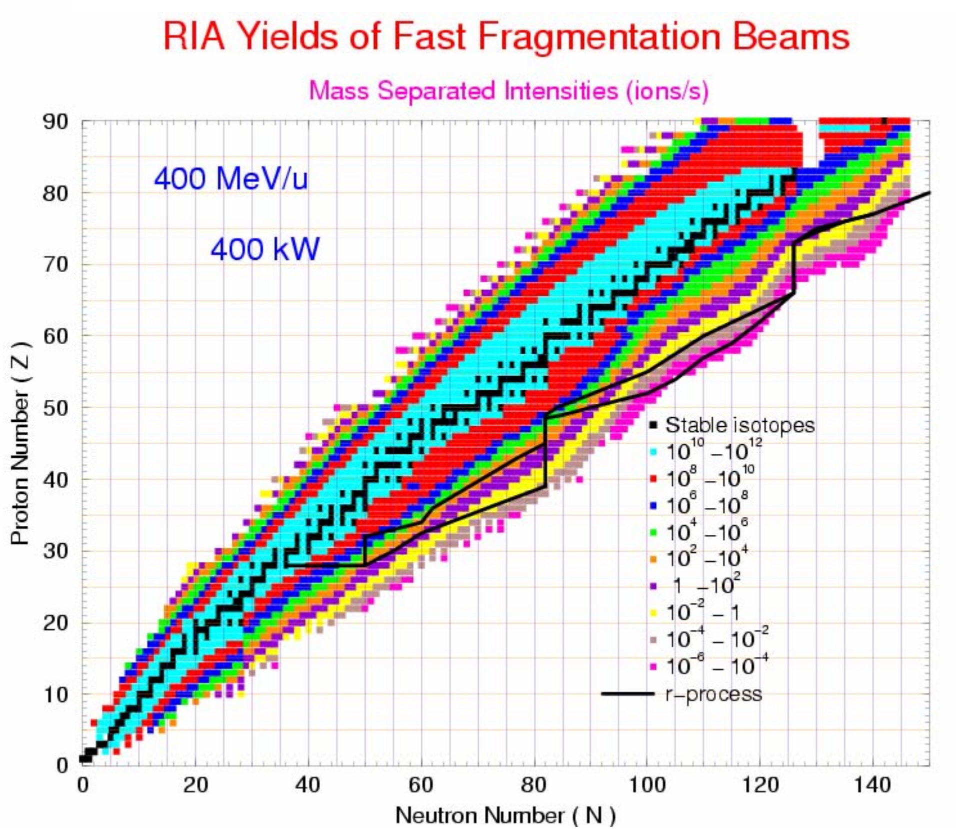
^{12}C(α,γ)^{16}O

^{44}Ti(α,p)^{47}V

PRL 84, 1651(2000)

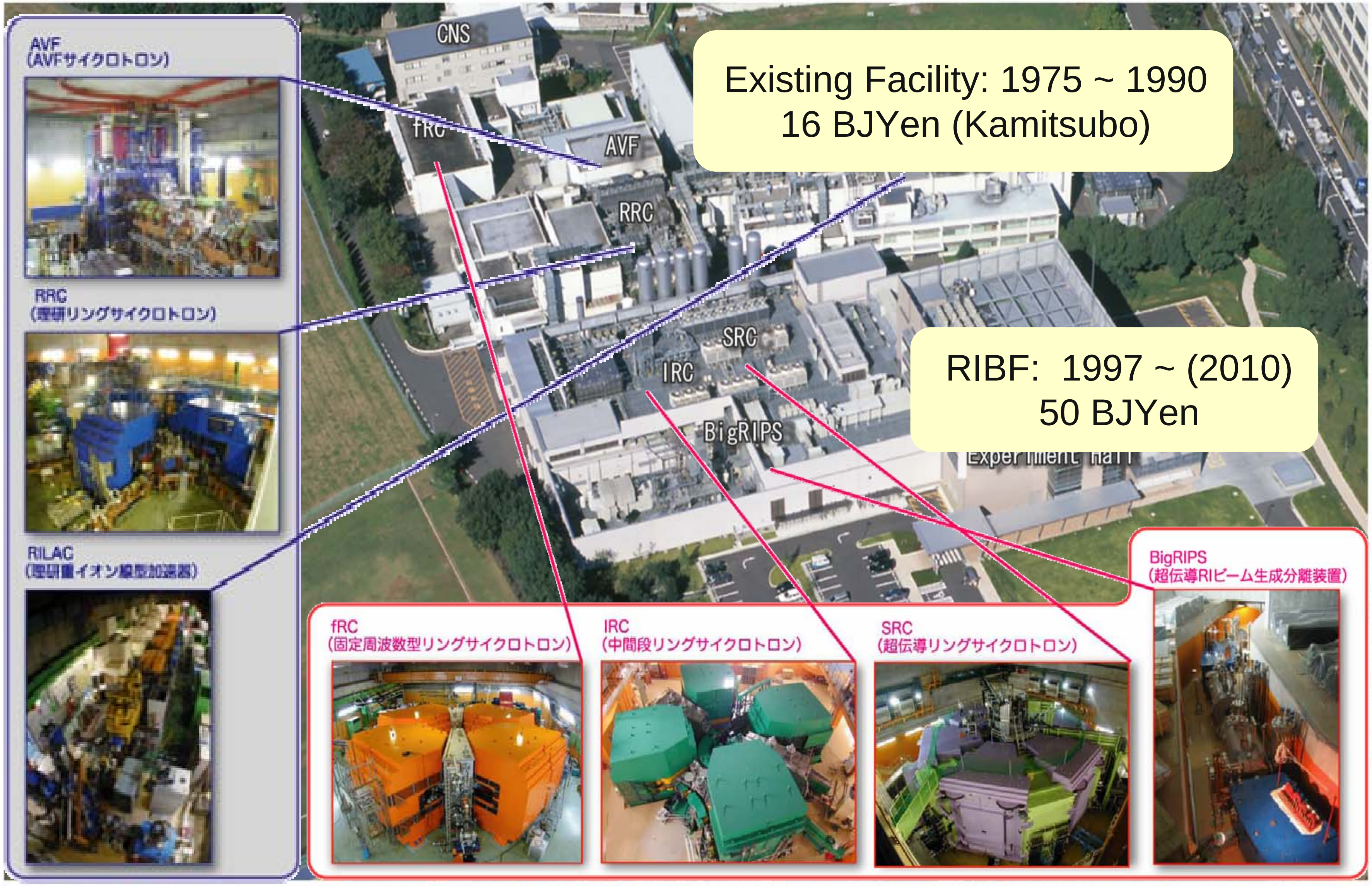
Radioactive beam intensities from an advanced facility such as RIA





See www.phy.anl.gov for predicted yield of every isotope

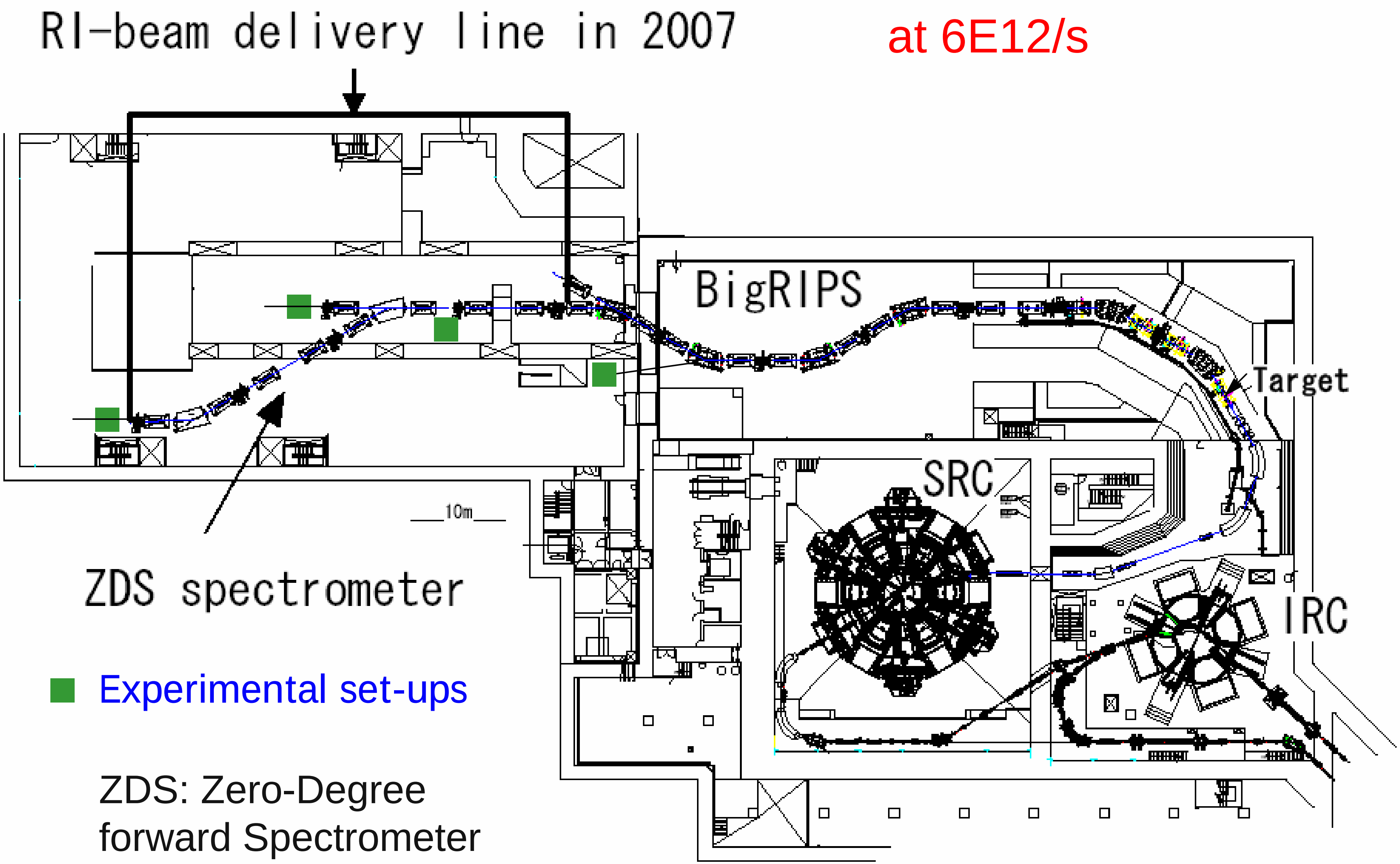
RIKEN RI Beam Factory (RIBF), Nishina Center, Wako-city



Prof. Y. Yano, CAARI, 2006

RIBF layout in 2007

Production beams up to 350 MeV/u uranium at 6E12/s



■ Experimental set-ups

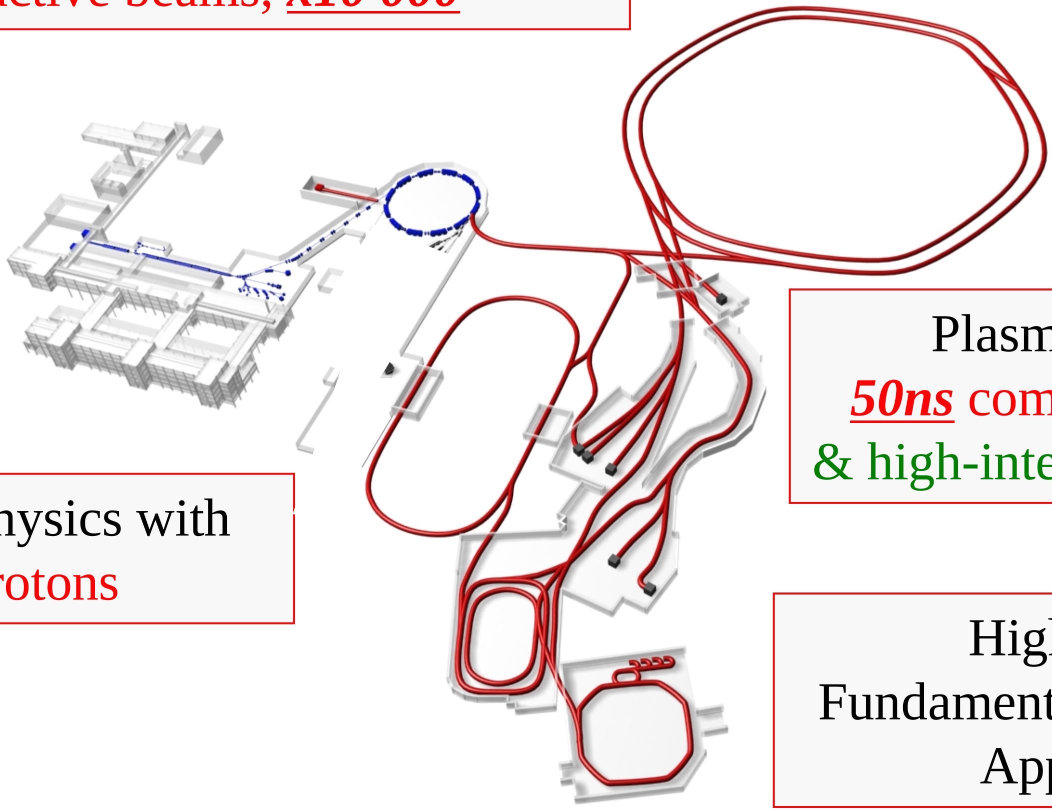
ZDS: Zero-Degree forward Spectrometer

Overview of Research at FAIR

Nuclear Structure & Astrophysics with
radioactive beams, ***x10 000***

Nuclear Matter Physics with
35-45 GeV/u HI beams, ***x1000***

Phase 1 ~2011,
complete ~2015



Plasma Physics with
50ns compressed ion beams
& high-intensity petawatt- laser

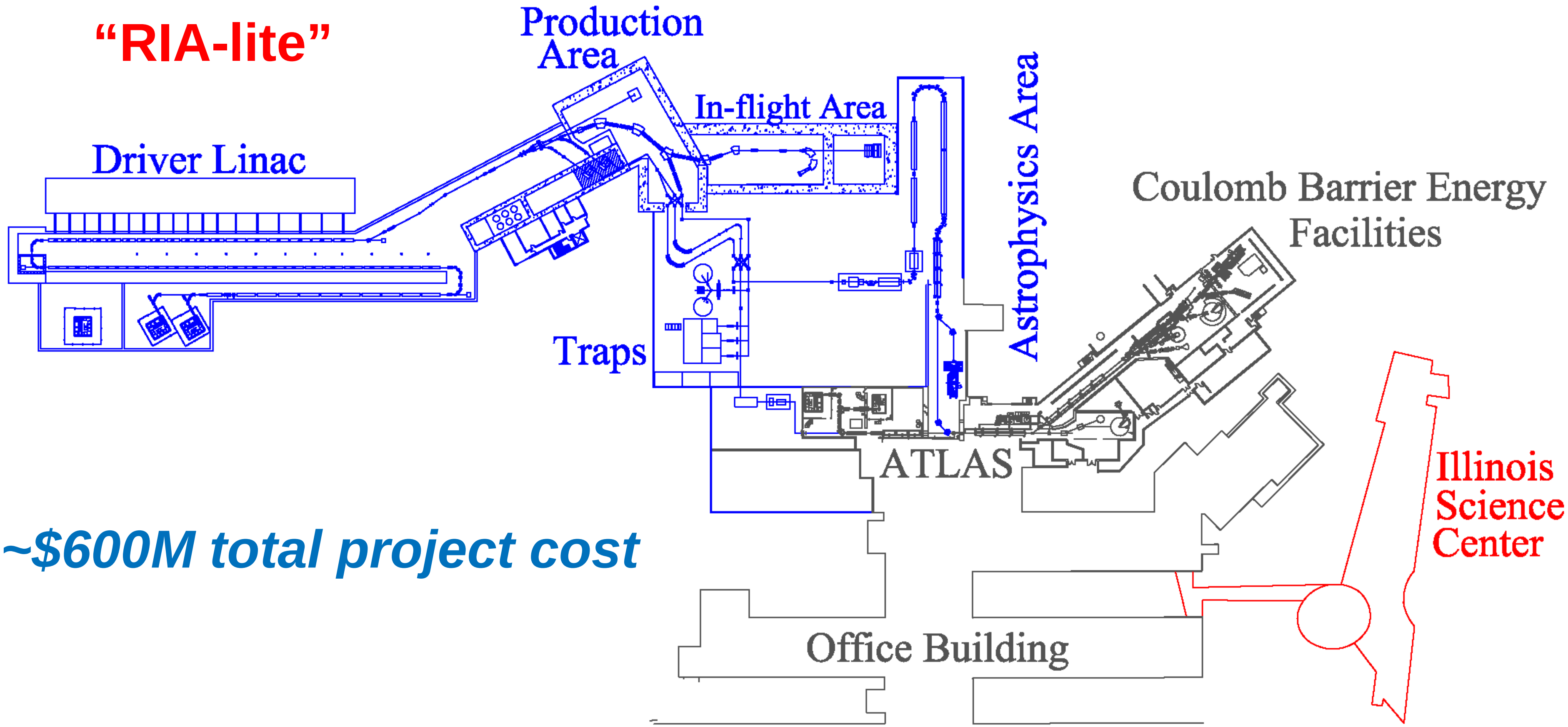
Hadron Physics with
antiprotons

High EM Field (HI)
Fundamental Studies (HI & p)
Applications (HI)

100 m

Preliminary plan for the AEBL facility at Argonne

"RIA-lite"



~$600M total project cost

Driver beam power 400 kW, 550 MeV protons to 200 MeV/u uranium

AEBL driver - Beams for one-strip option:

Driver Linac - Beam Parameters (200 MeV/u option)

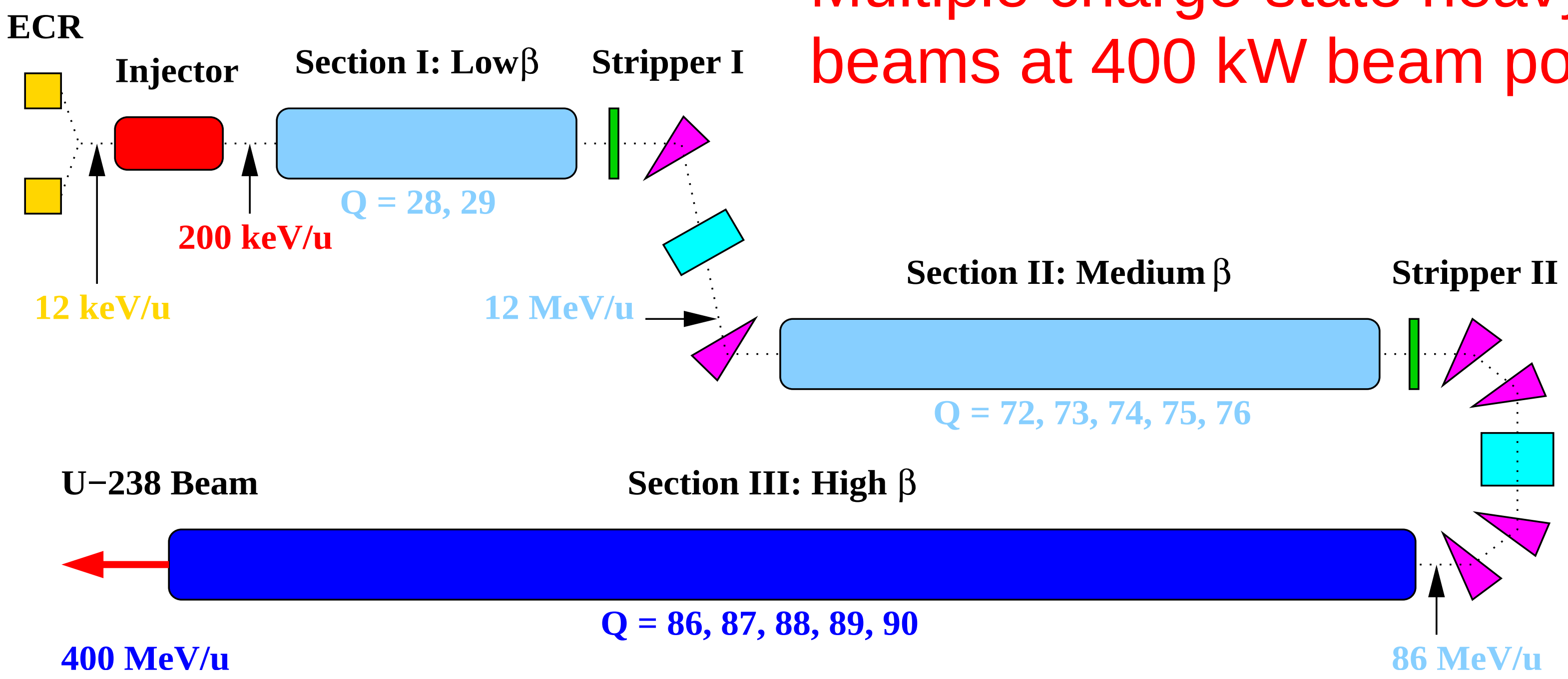
(Assumes 80% bunching efficiency, 4% energy loss in the second stripper, required ECR performance)

		-------ECR-------		Stripper			OUTPUT BEAM		
Z	A	I source pmicroA	Qinj	Energy MeV/A	Qstrip	Frac	I out pmicroA	Energy MeV/A	Power kW
1	1	880	1	95.2	-	-	704.1 (p: 4E15/s)	568	400
2	3	390	2	70.7	-	-	312.4	427	400
1	2	728	1	57.1	-	-	582.0	344	400
8	18	101	6	41.8	8.0	0.90	72.9	305	400
18	40	47	8	27.6	18.0	0.90	33.7	297	400
36	86	24	14	23.0	35.0	0.90	17.5	266	400
54	136	17	18	18.9	50.7	0.90	12.4	237	400
92	238	6 *	28-29	17.0	79.0	0.83	8.4 (U: 5E13/s)	200	400

* single charge state

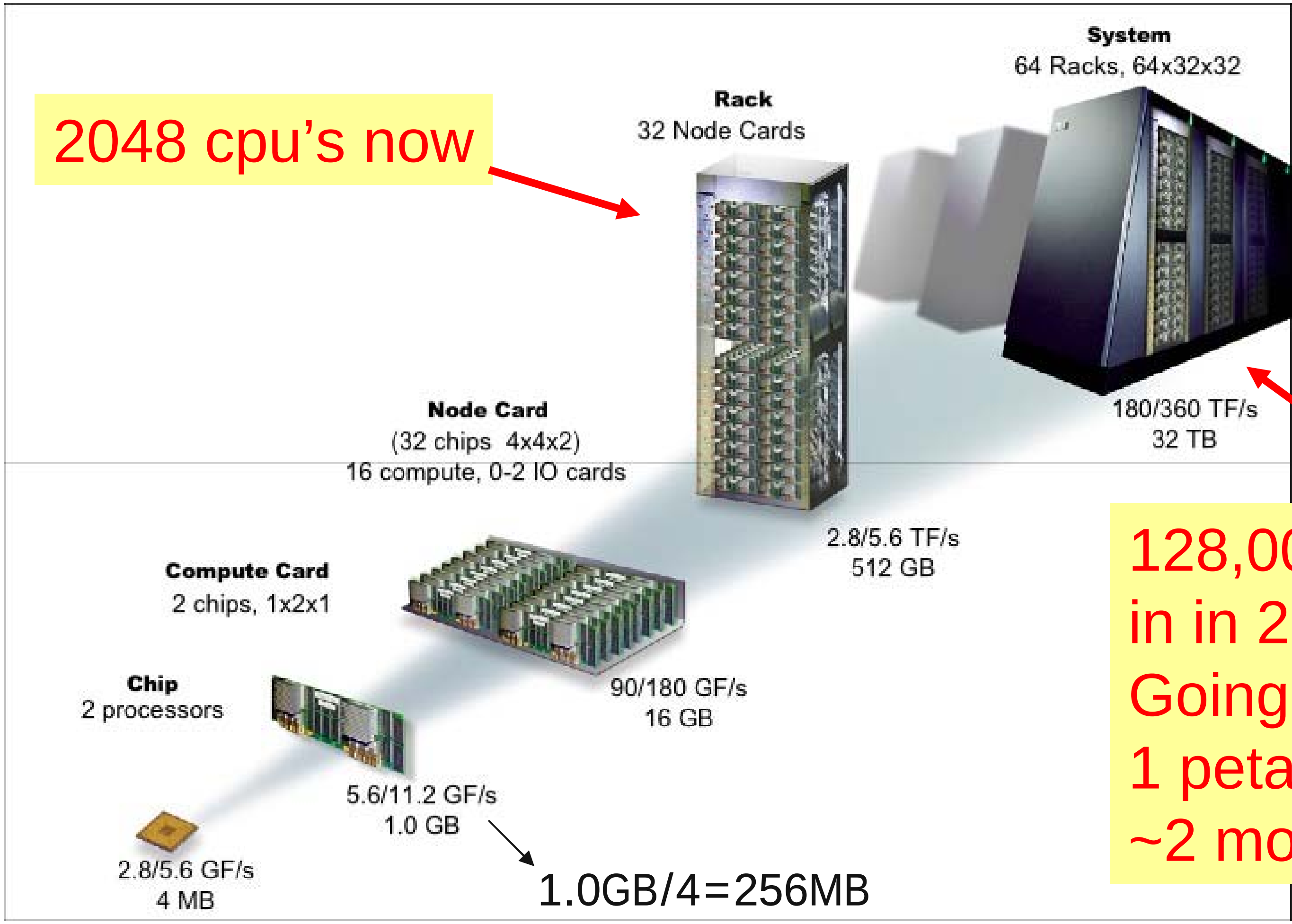
Layout of the full RIA Driver Linac

Multiple charge-state heavy ion beams at 400 kW beam power



Baseline: About 1200 beam line elements: ~ 300 rf resonators, 90 solenoids, 100 quads, 16 bending magnets, …

BlueGene/L and more at Argonne



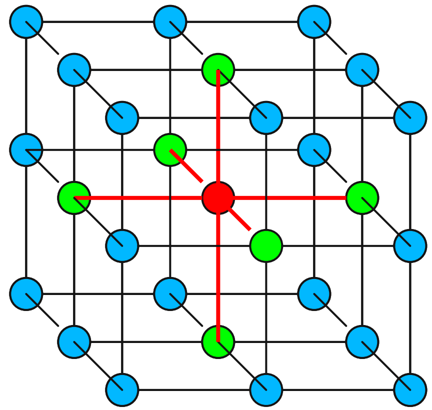
128,000 cpu's
in in 2007;
Going to
1 peta-flop/s in
~2 more years

Future accelerators could have dedicated peta-scale computing.

BlueGene architecture

Three-Dimensional Torus – point-to-point

The Torus network is used for general-purpose, point-to-point message passing.



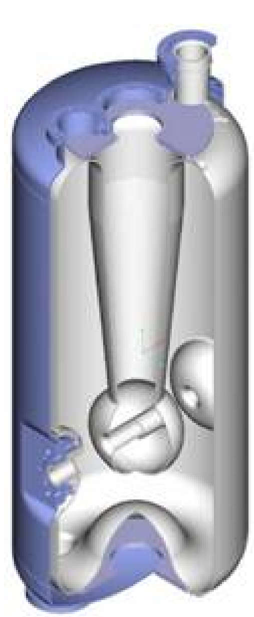
The topology is a three dimensional torus constructed with point-to-point. Therefore, each ASIC has six nearest neighbor connections.

The target hardware bandwidth for each Torus link is 175 MB/s in each direction for link for a total of 2.1 GB/s bidirectional bandwidth per node.

Large-scale simulation needs for design optimization

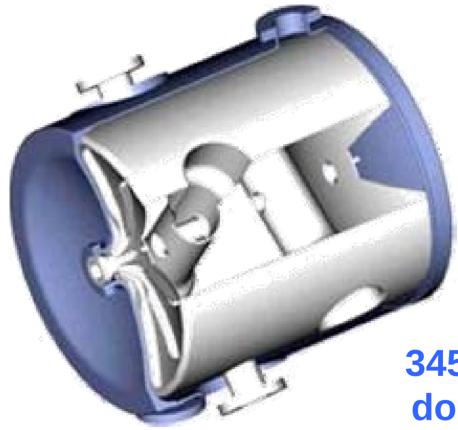
- Complex magnet and RF cavity design
  - Detailed 3D electromagnetic models are essential to adequate beam dynamics simulations
- Detailed beam halo and loss sensitivity to alignment and parameter uncertainties are required
- Space-charge tracking, possibly implemented via 3D Vlasov solver (Berz talk tomorrow)
- Detailed determination of the necessary diagnostics information to ensure adequate instrumentation
- Shielding and activation models integrated with the beam halo and loss simulations
- Fragment separator resolving power optimization coupled to radiological heating, activation, and damage minimization
- Use of rigorous global optimization (Makino talk yesterday)

SC cavities covering the velocity range 0.12 < β < 0.8 (all designed at Argonne by Ken Shepard using Microwave Studio)

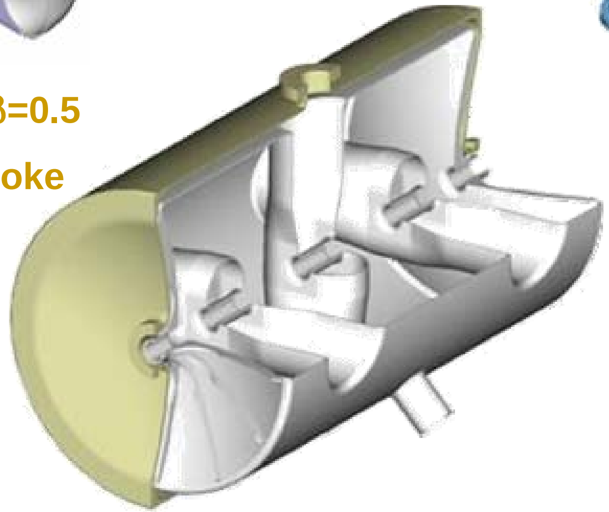


115 MHz β=0.15 Steering-corrected QWR

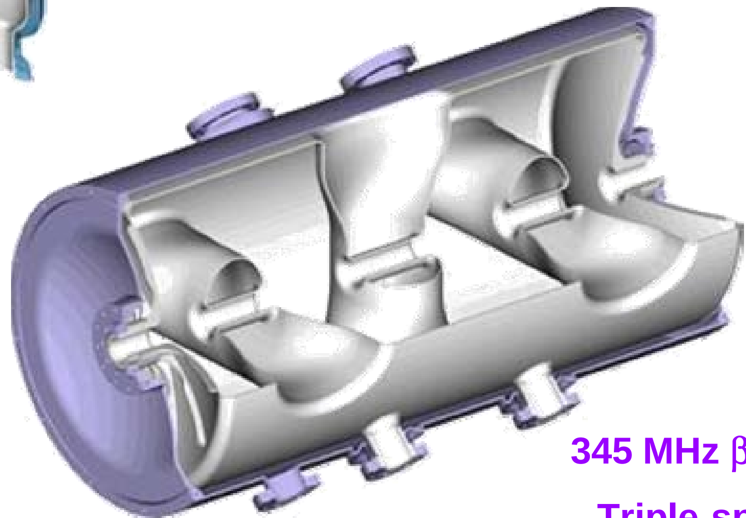
172.5 MHz β=0.28 HWR



345 MHz β=0.4 double-spoke



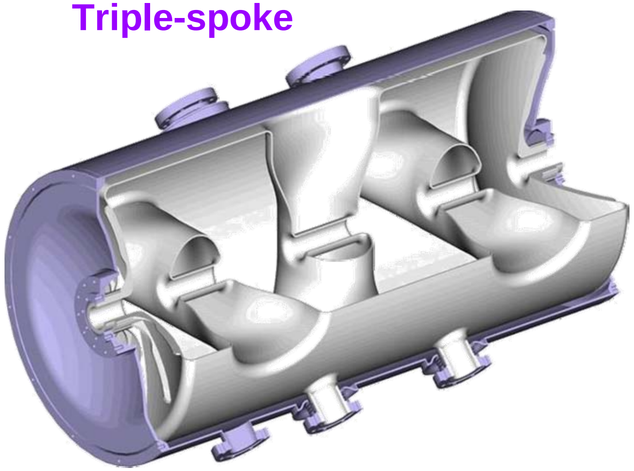
345 MHz β=0.5 Triple-spoke

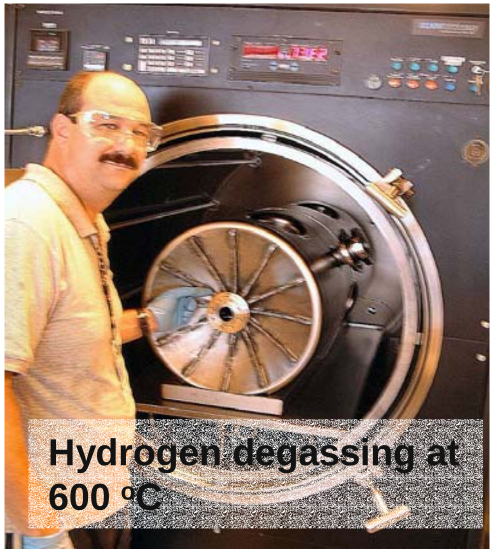


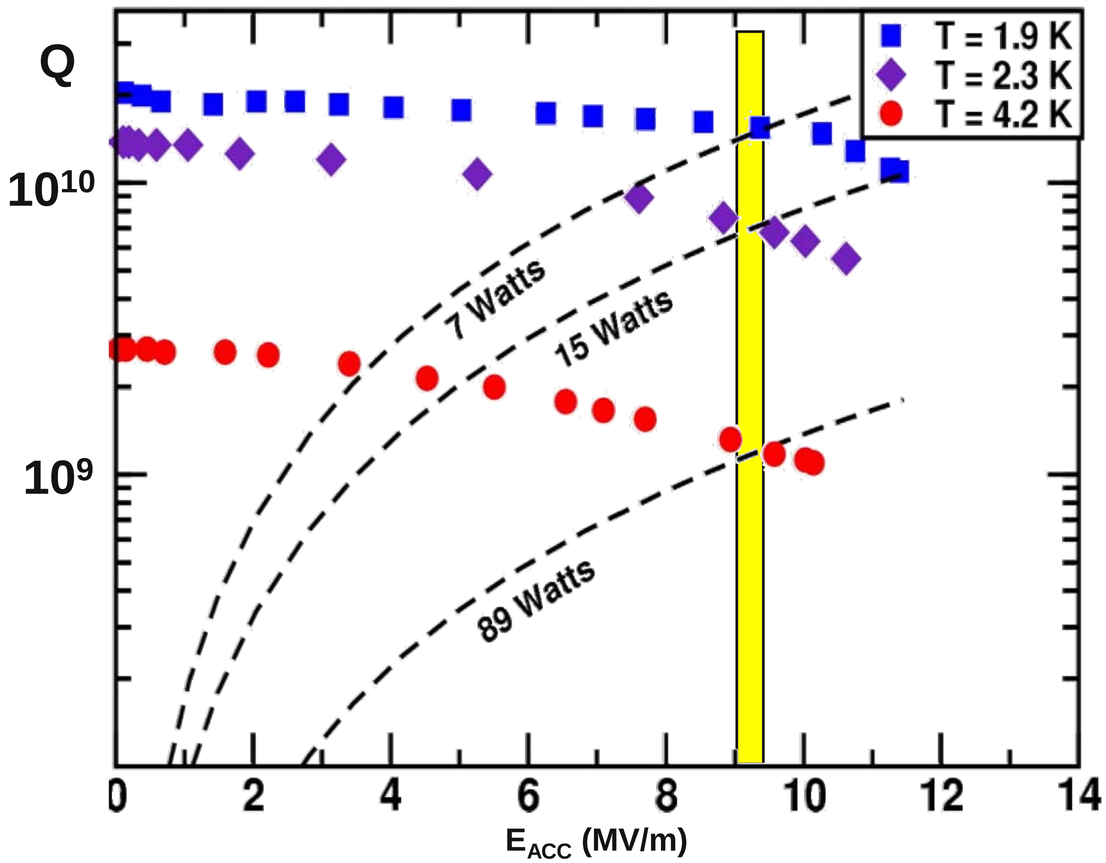
345 MHz β=0.62 Triple-spoke

High-performance mid-β multi-spoke superconducting cavities developed at Argonne

345 MHz β=0.63
Triple-spoke







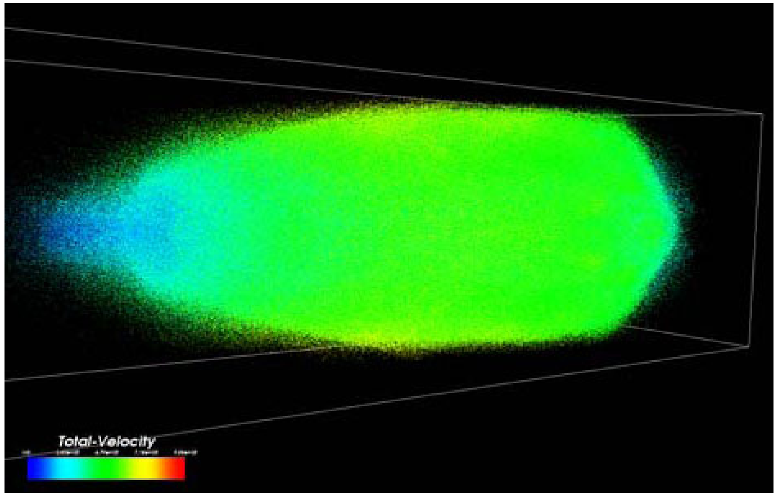
Ken Shepard and Mike Kelly
PAC2005, Knoxville, TN, TPPT099, TPPT100, May 16-20, 2005.
SRF2003, TuP53, Travemunde, Germany, Sept. 8-12, 2003.

TRACK: Developed for particle tracking with space charge through all RIA elements

- Multiple charge-state ion beams
- Any type of RF resonator (3D E&B fields)
- Static ion-optic devices (3D fields)
- Radio-Frequency Quadrupoles
- Solenoids with fringe fields
- Bending magnets with fringe fields
- Electrostatic and magnetic multipoles
- Multi-harmonic bunchers
- Axial-symmetric electrostatic lenses
- Entrance and exit of HV decks
- Accelerating tubes with DC voltage
- Transverse beam steering elements
- Stripping foils or film
- Horizontal and vertical jaw slits

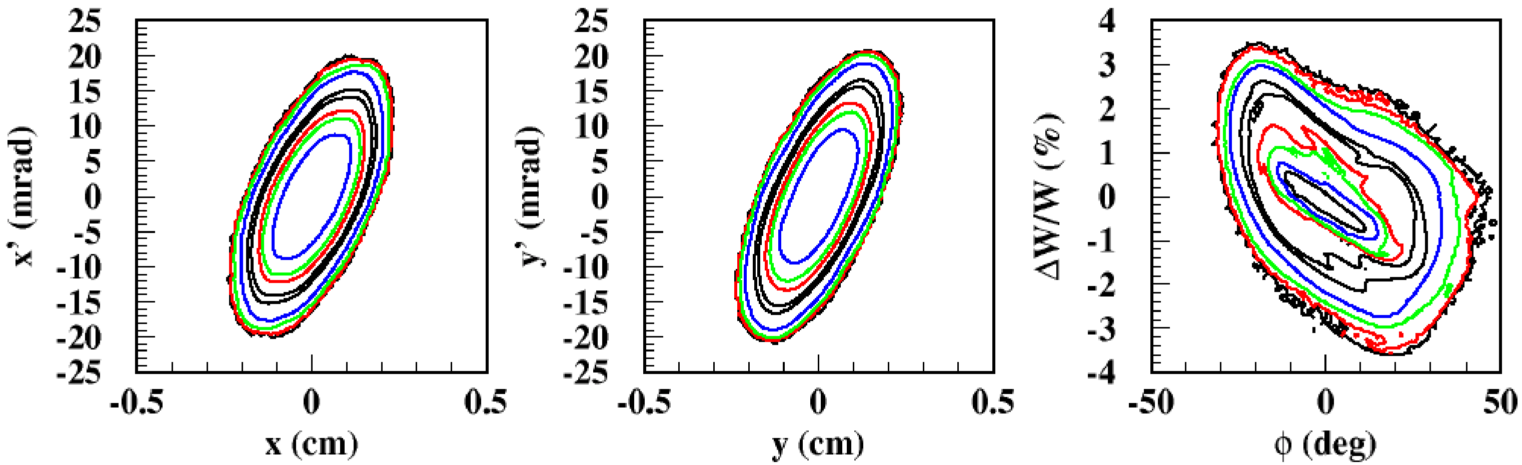
P. Ostroumov, V. Aseev, and B. Mustapha

Tracking of every particle in a 40 mA bunch through an RFQ with TRACK and 1024 processors on BlueGene/L at Argonne (18 hrs)



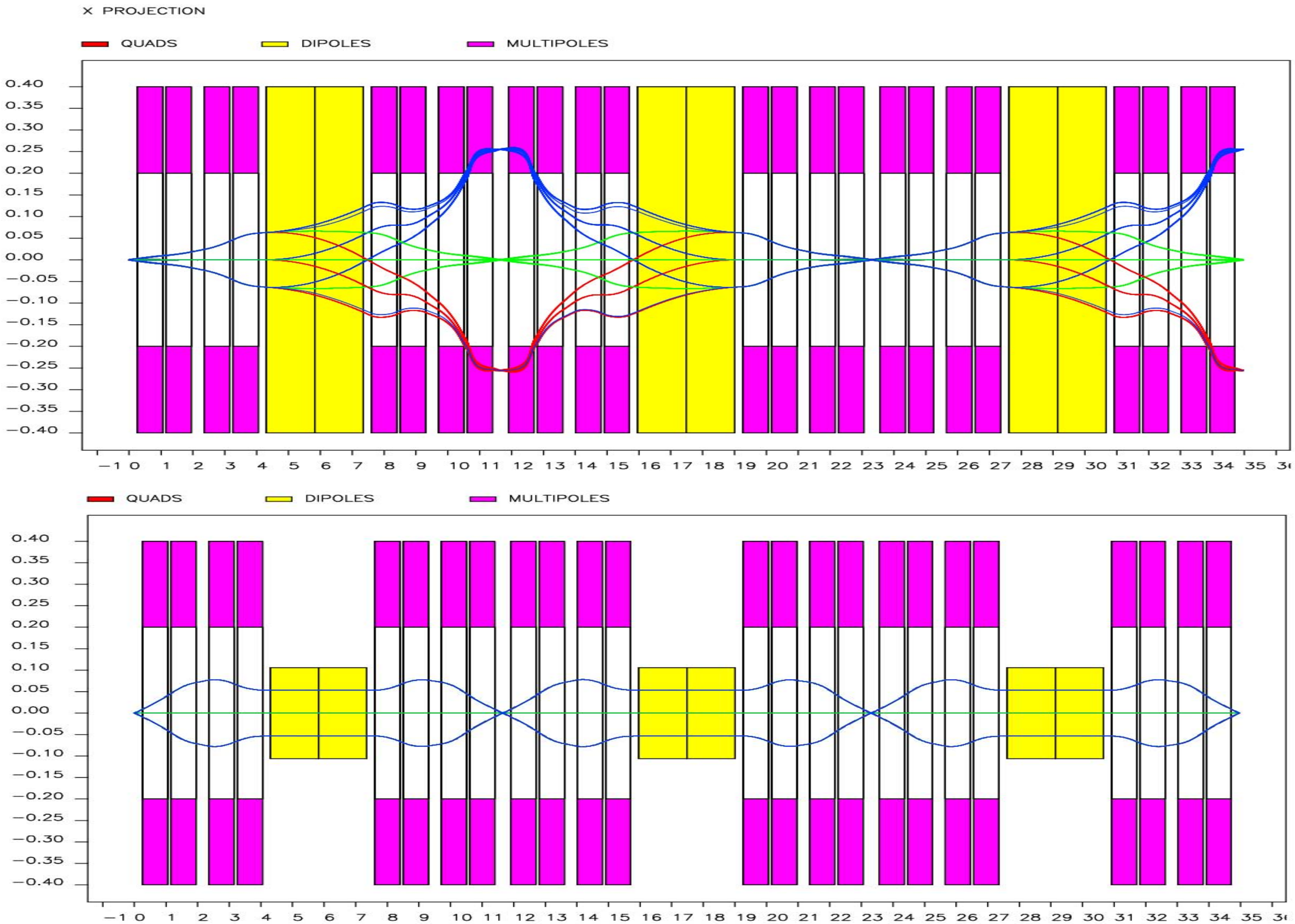
100 million particles in a 3D bunch (display by ANL/MCS visualization group).

2D projections of the 1E8 ions.



J. Xu, P. Ostroumov, V. Aseev, and B. Mustapha

Large acceptance fragment separator design and optimization using COSY Infinity with new extensions



What was not in COSY?

- No nuclear physics
- No beam-material interactions
- No stochastic processes
- Everything is relative to a reference particle
  => no global coordinate system available

But these are needed for Fragment Separator design

Work by B. Erdelyi and students (NIU and Argonne) with help from M. Berz, K. Makino, and students at MSU.

Coming soon: Large aperture magnet maps with 3D field solver – S. Manikanda paper from Monday.

Nuclear Physics in COSY

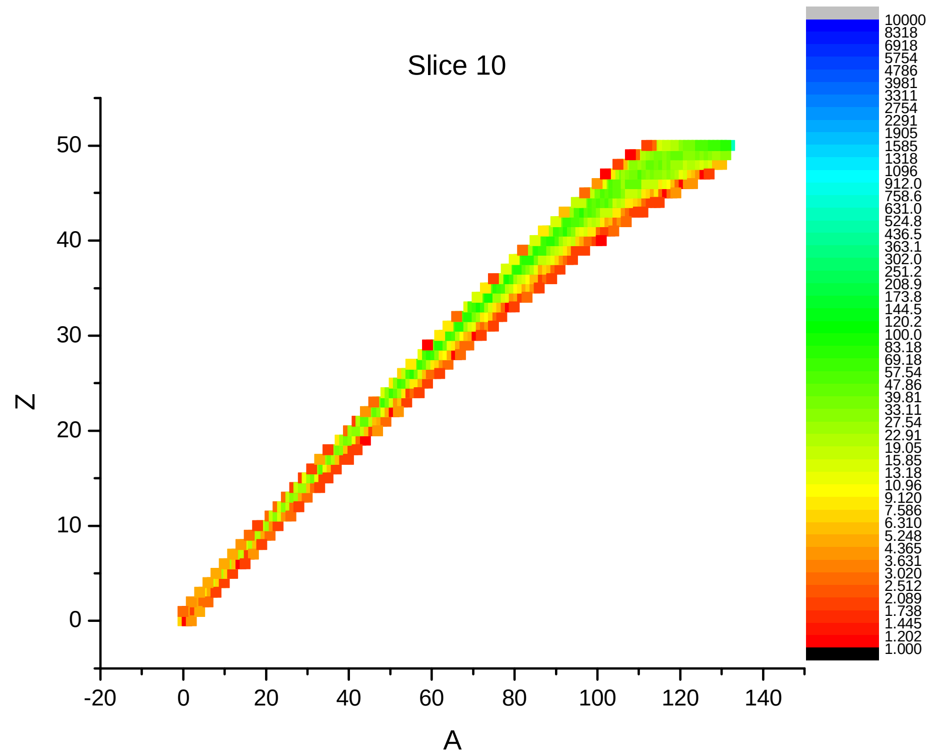
- The functionalities of the following codes have been added to COSY (now intrinsic functions callable from within COSY's own language):
  - ***EPAX 2.1****: fragmentation cross-sections*
  - ***GLOBAL****: charge state distributions*
  - ***ATIMA****:*
    - energy loss
    - energy straggling
    - angular straggling

NOTE: We use the version of ATIMA based on splines, i.e. for each projectile-target combination, there is a spline file, containing the splines that give the range as a function of initial energy, and the standard deviations for the straggling => about 250 MB of data, but fast

Integrated Approach to Nuclear Processes and Beam Optics Design

- **State of the art beam optics code (COSY INFINITY)**
- **A suite of nuclear physics codes (ATIMA, GLOBAL, EPAX)**
- **Work seamlessly together to allow accurate and fast design work**
  - **Map mode for optimization**
  - **Hybrid Monte-Carlo mode for simulations**

- **End-to end simulations**
- **Layout, magnet strengths, target thickness, and wedge shape optimization**
- **All particles, including background, can be followed through the system**
- **Effects of multiple fragmentations can be studied**



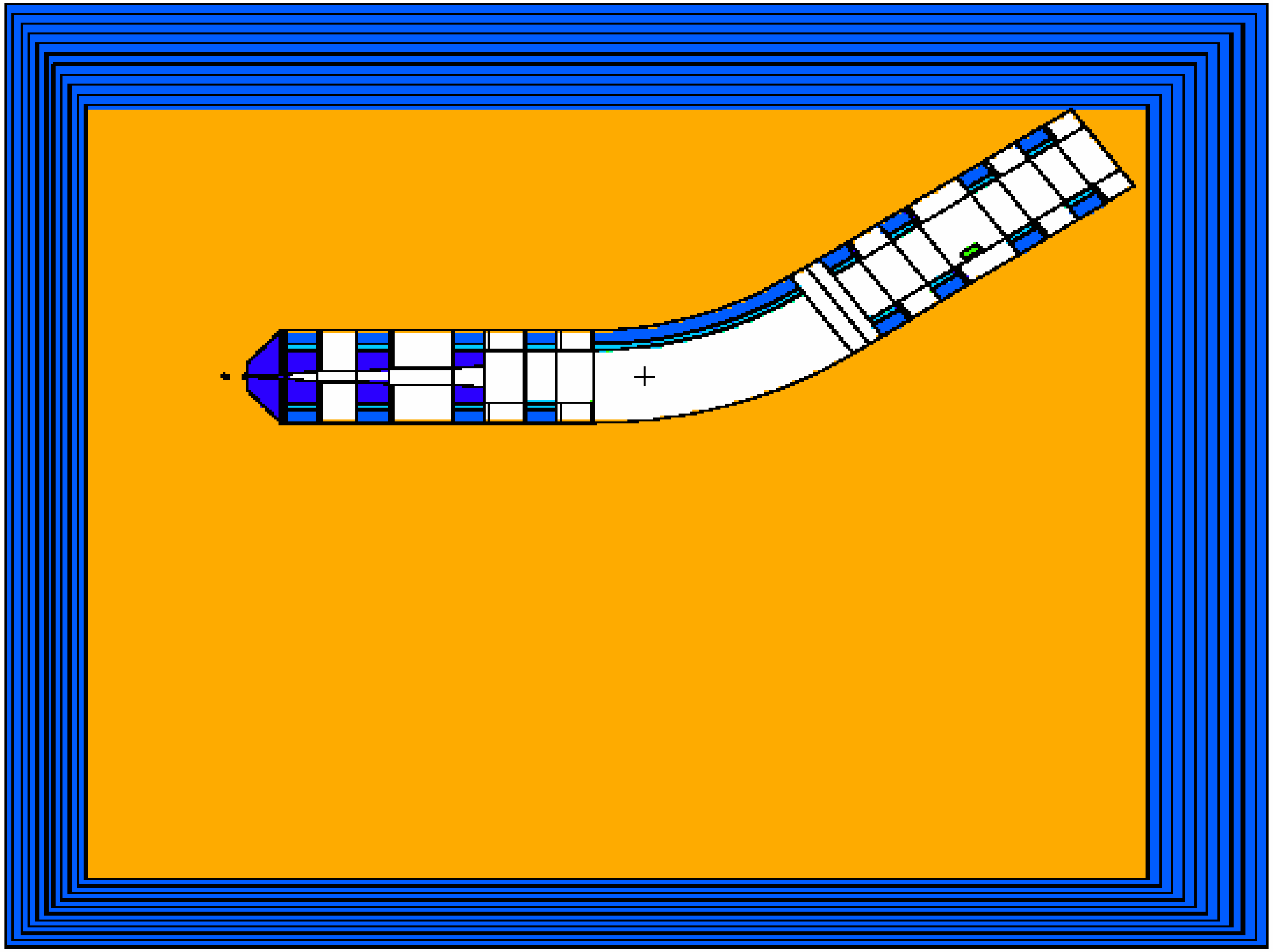
Ions can fragment in layers of the target & wedges – many secondaries possible.

Computational Challenges

- **Magnitude of the optimization problem:**
  - **Basic optics:**
    - Drift lengths
    - Magnet strengths
    - Number and location of multipole correctors
  - **Advanced optics**
    - Accurate transfer maps based on detailed field maps, including fringe fields
    - Will incorporate 3D magnet field models developed by Manikonda, Berz, & Makino
  - **Energy degraders:**
    - Thickness
    - Shape
  - **Integrated beam optics - nuclear physics simulations**
    - Tracking of thousands of isotope species
    - Total number of particles tracked in the billions range due to low cross-section of particles of interest

Beam optics codes need to be integrated with Monte Carlo particle tracking through materials for radiological effects (MCNPX)

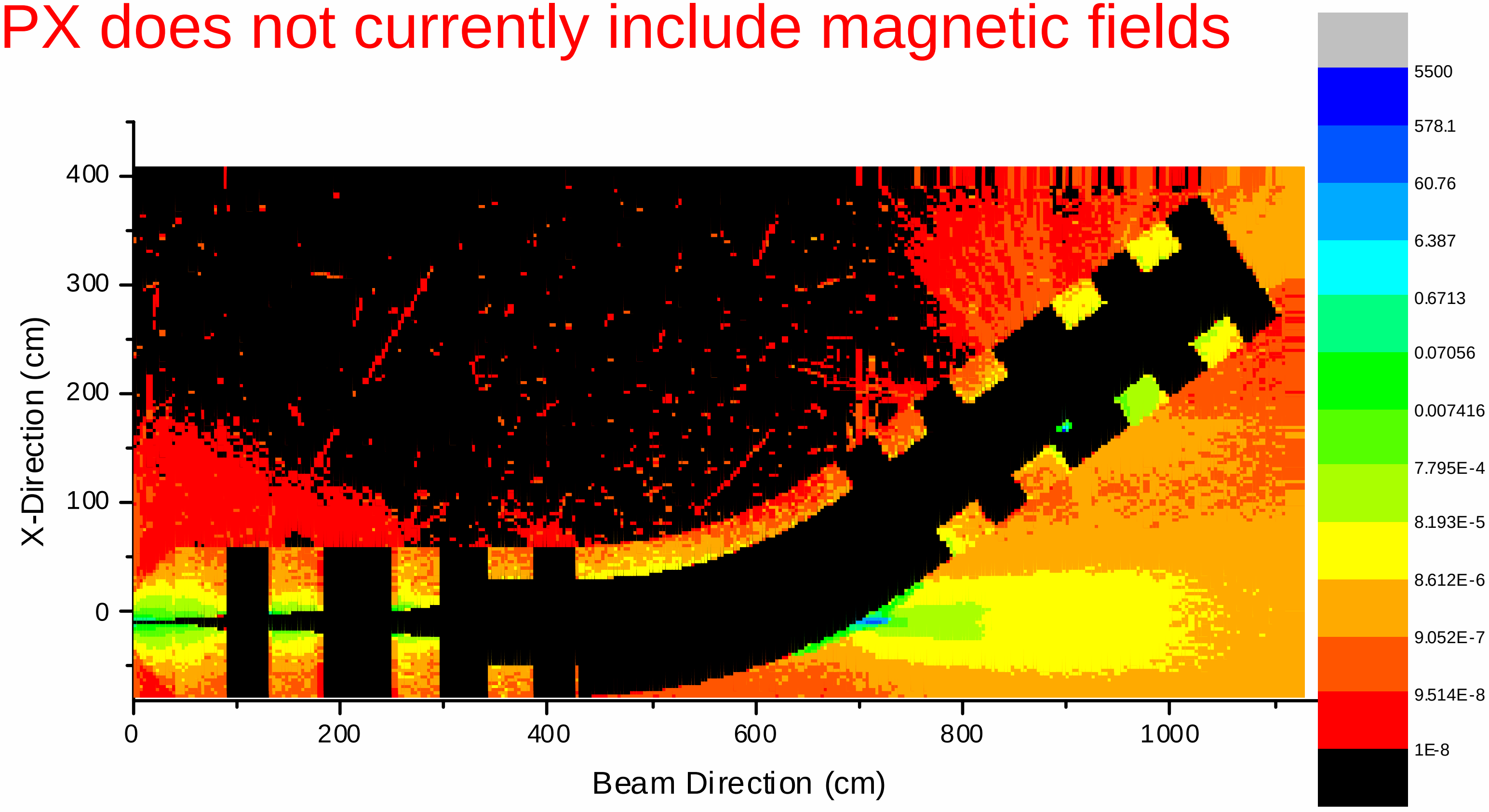
MCNPX Model of the Fragment Separator and Fragmentation Target (radiological issues)



I.C.Gomes

Calculated Heat Deposition (MeV/cc per particle) using MCNPX on the NERSC Seaborg cluster

MCNPX does not currently include magnetic fields



I.C.Gomes Consulting & Investment Inc

Large-scale computations applied to operation: "A Model-Driven Accelerator"

- On-line peta-scale computing is needed for near real-time tune optimization based on diagnostics feedback and detailed facility model
- Such capability would greatly improve operational efficiency and reliability
- There are many challenges here, such as determining the requirements and providing an adequate set of diagnostics information, the time response and accuracy of the diagnostics information, the validation of the hardware calibrations with the model parameters, and the integration of the model simulations with the diagnostics information and the control system.

Summary & future developments

- Tera-flop-scale simulations of many aspects of accelerator facilities are currently fairly routine.
- Further integration of codes to enhance the optimization processes will continue with consideration of scalability to peta-flops/s in the coming years.
- Full integration of detailed accelerator models, feedback from diagnostics devices, and control systems has the potential to greatly improve operational efficiency and reliability of future facilities