High-Order Achromatic Optics for FRIB Fragment Separators: Transfer Maps, Differential Algebraic Methods and Symmetries

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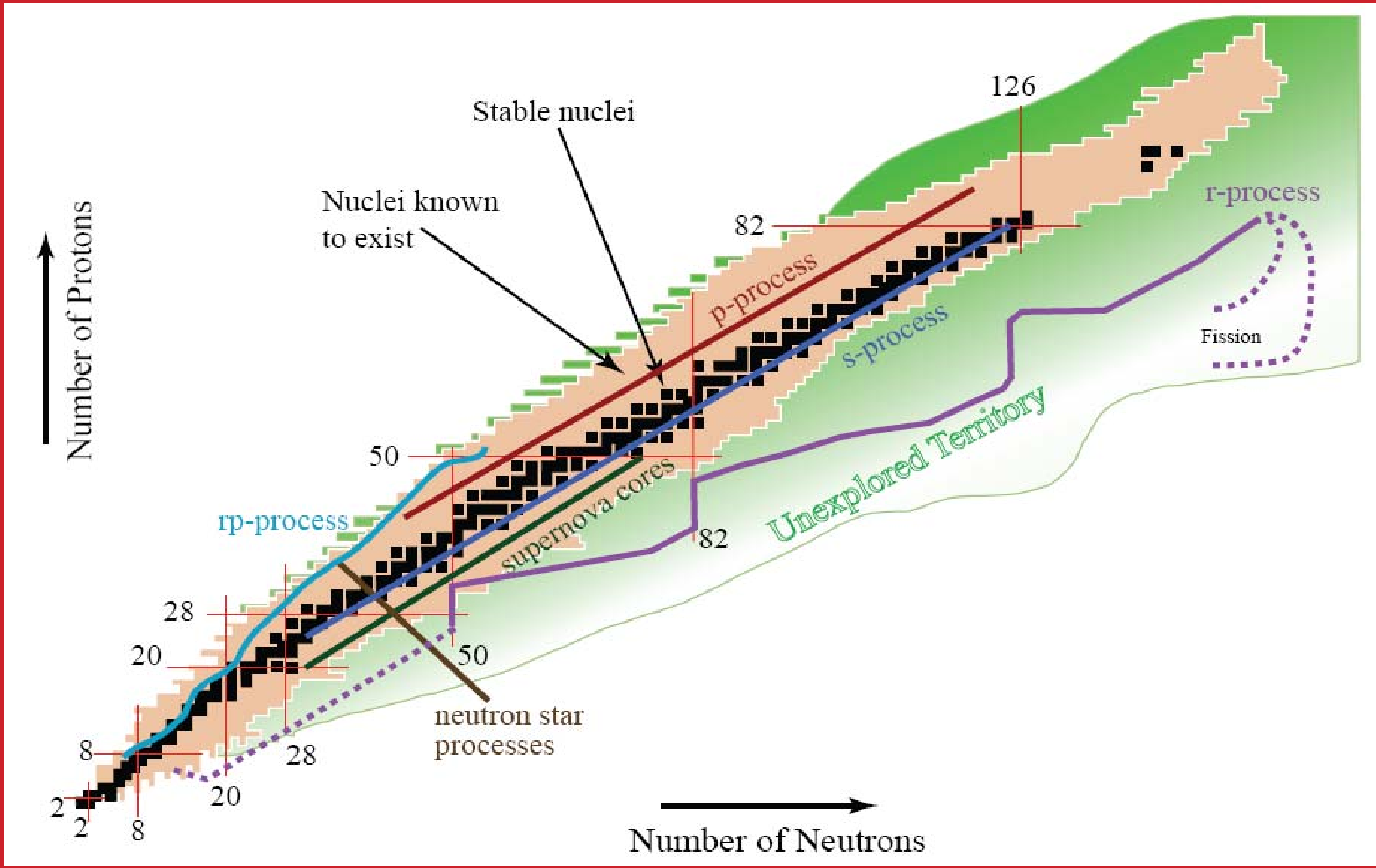
Outline

- **Introduction**
  - What are rare isotopes?
  - Why and how are they produced?
  - Overview of FRIB
- **Codes for design and simulations**
  - General overview
  - COSY Infinity: transfer maps and Differential Algebra (DA)
  - New integrated framework
- **Results**
  - Design optimization: symmetries and achromatic optics
  - System performance

What are Rare Isotopes?

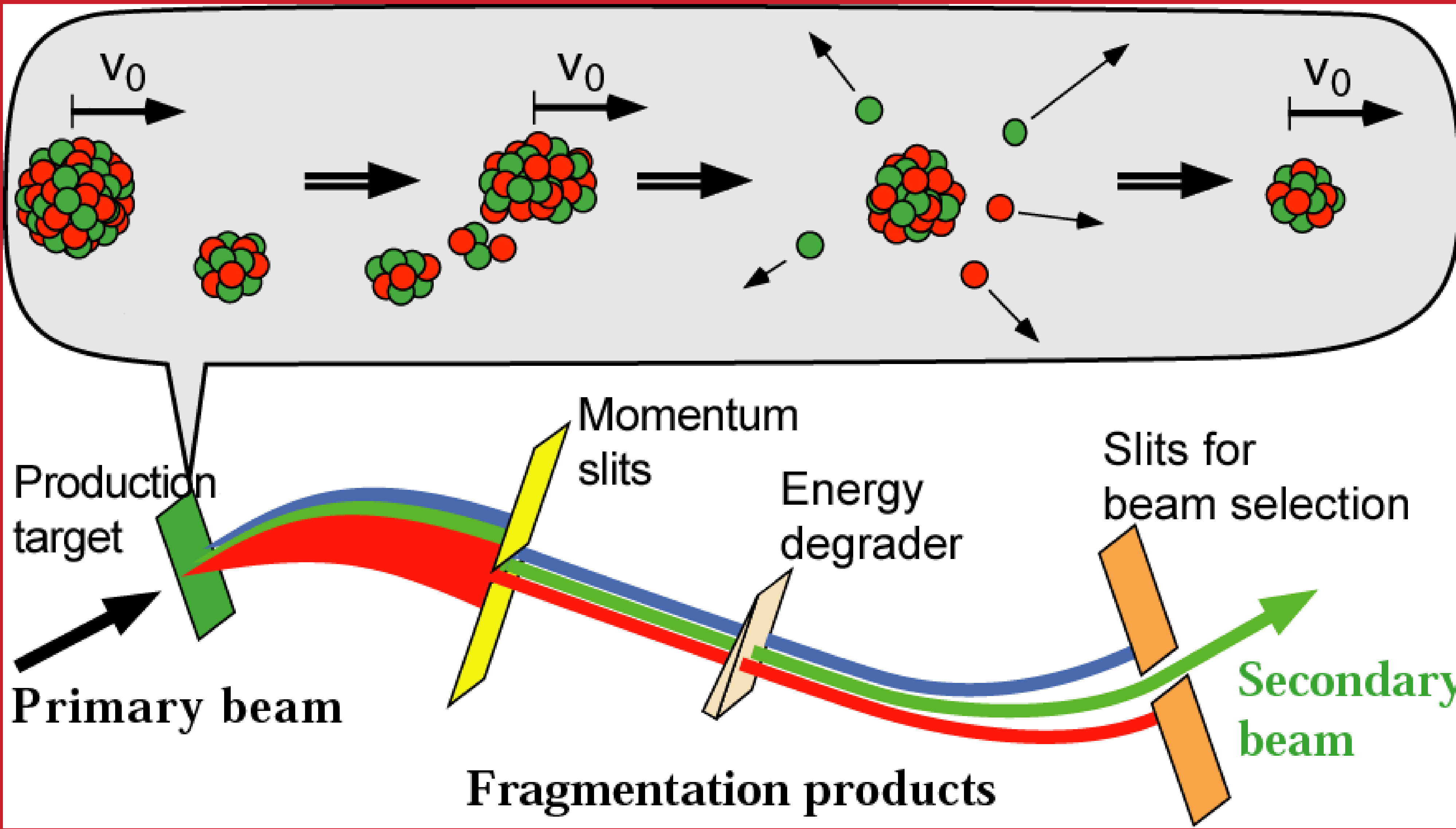
- Isotopes of elements far from the valley of stability
- Unstable, proton- or neutron-rich
- Very important in basic and applied science



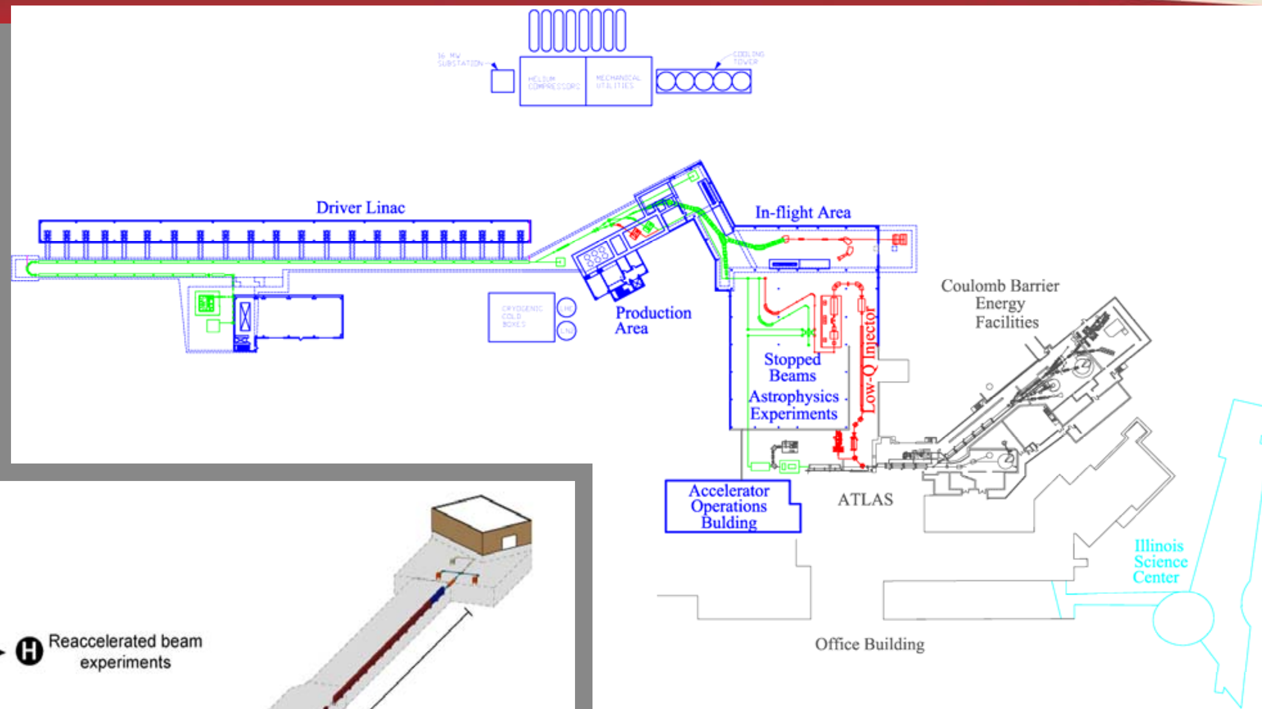
What Are Radioactive Beams Good For?

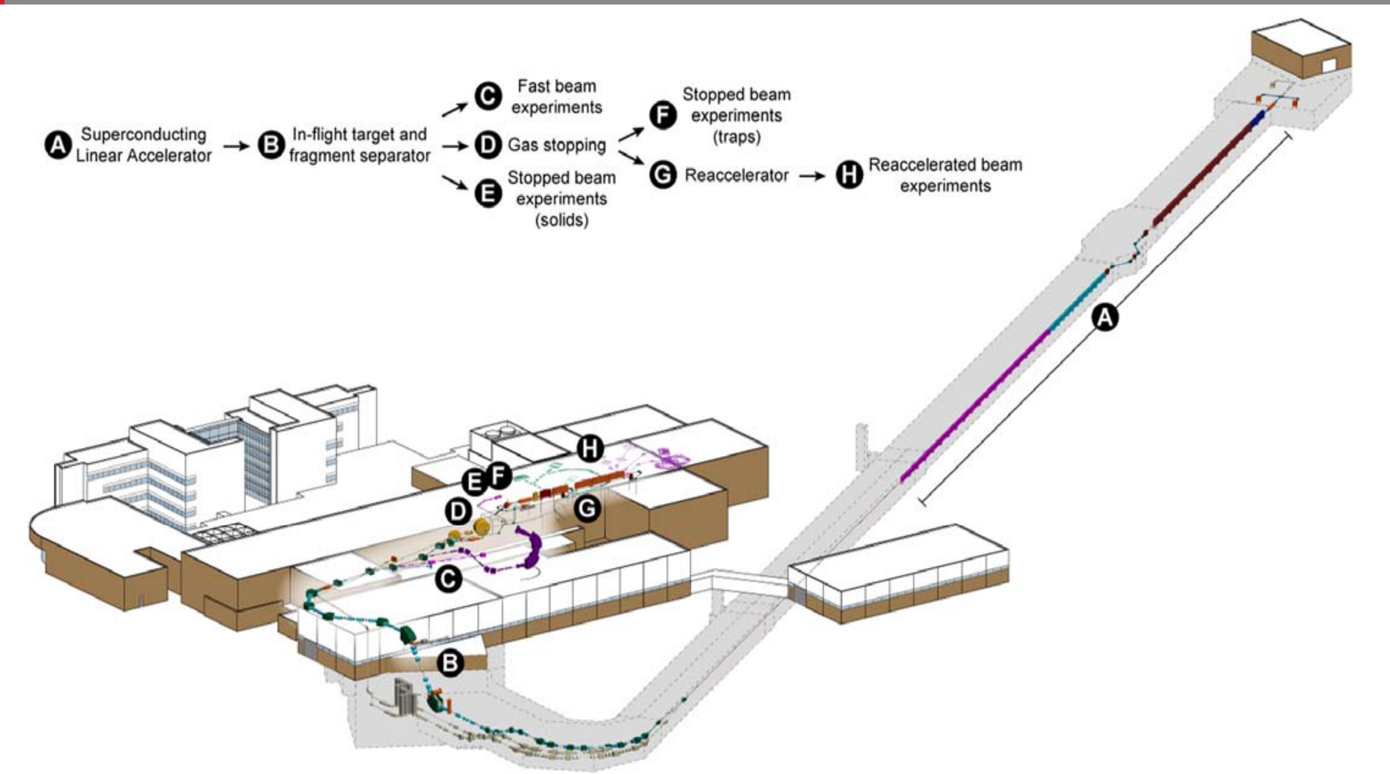
- **Physics of Nuclei**
  - How do protons and neutrons make stable nuclei and rare isotopes?
  - What is the origin of simple patterns in complex nuclei?
  - What is the equation of state of matter made of nucleons?
  - What are the heaviest nuclei that can exist?
- **Nuclear Astrophysics**
  - How are the elements from iron to uranium created?
  - How do stars explode?
  - What is the nature of neutron star matter?
- **Fundamental Interactions**
  - Why did the Big Bang produce more matter than antimatter?
  - What are the weak interactions among hadrons, and how are they affected by the nucleus?

Schematic of the Fragmentation Process

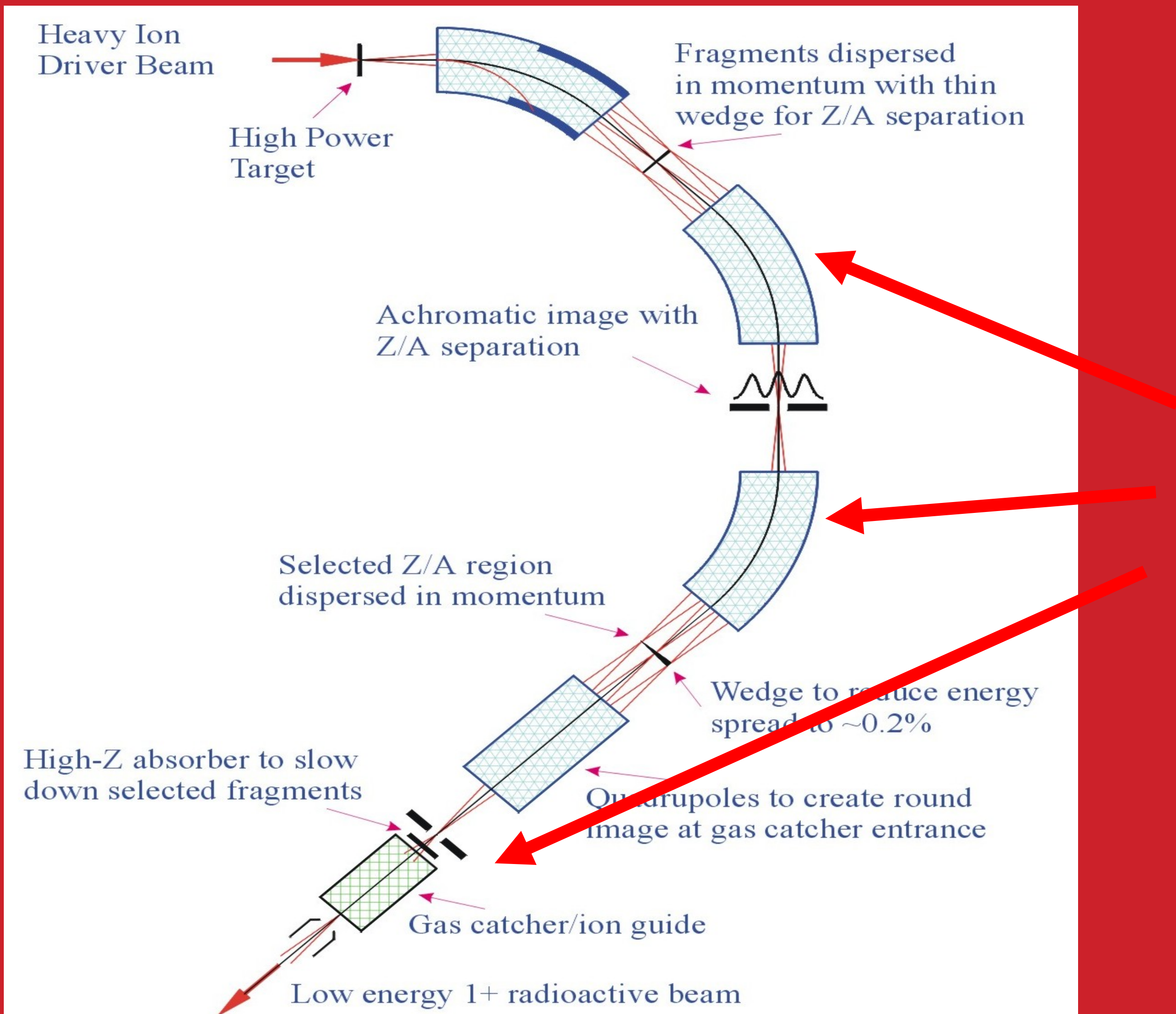


SCHEMATICS OF FRIBS





Schematic Layout of Fragment Separator Area



Schematic layout of fragment separator, achromatization stage and gas catcher system

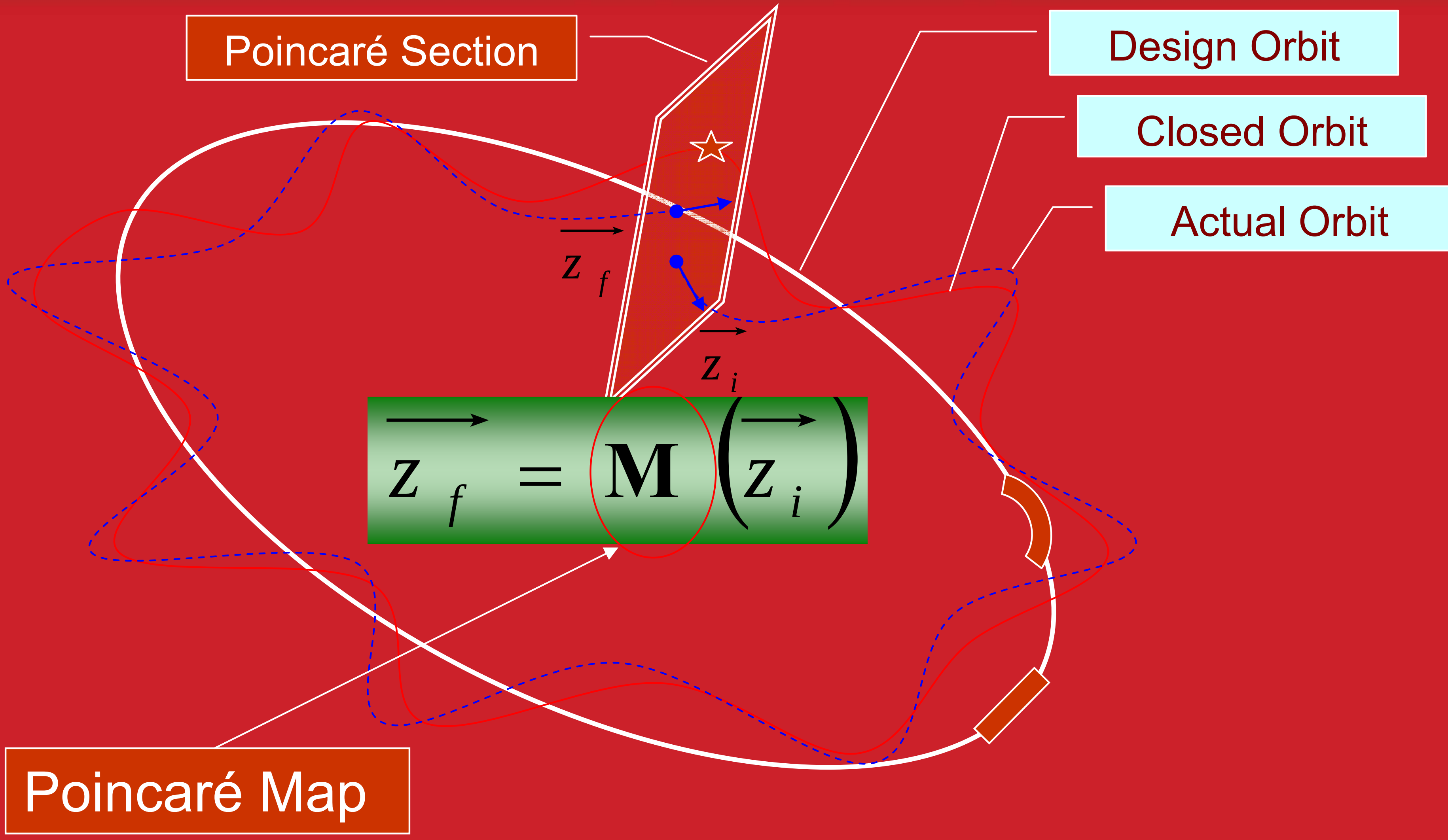
General Purpose Codes

- **Beam Optics**
  - COSY Infinity
  - GICOSY, GIOS
  - Transport
  - Marylie
  - Many others
- **Radiation transport**
  - MCNPX
  - MARS
  - PHITS
  - GEANT

Specialized for Fragment Separators

- **LISE++**
  - **MSU code**
- **MOCADI**
  - **GSI code**
- **Extensions of *COSY Infinity***
  - **Developed by us**

Mathematical Model of Periodic Accelerators



Computation of Derivatives

Differential Algebraic Methods

- Solve analytic problems by algebraic means
- Most important for beam physics is the computation of Taylor expansions of the flow of ODEs $\Longleftrightarrow$ accurate computation of very high order derivatives of multivariable functions
- Push perturbation theory to high orders and maintain accuracy
- The structure ${}_1D_1$(for first derivative of a function of one variable) is defined as

$$(q_0, q_1) + (r_0, r_1) = (q_0 + r_0, q_1 + r_1)$$
$$t \cdot (q_0, q_1) = (tq_0, tq_1)$$
$$(q_0, q_1) \cdot (r_0, r_1) = (q_0 r_0, q_0 r_1 + q_1 r_0)$$

- It follows that

$$(f(x), f'(x)) = f(x + d)$$
$$d = (0, 1)$$

Differential Algebraic Methods: Example

$$f(x) = 2x^2 - x + 3$$
$$f'(x) = 4x - 1$$

$$f(2) = \mathbf{9}$$
$$f'(2) = \mathbf{7}$$

$$\begin{aligned} f(2+d) &= f(2,1) \\ &= 2(2,1)\cdot(2,1) - (2,1) + (3,0) \\ &= 2(4,4) - (2,1) + (3,0) \\ &= (8,8) - (2,1) + (3,0) \\ &= (\mathbf{9}, \mathbf{7}) \end{aligned}$$

Differential Algebra

- **An algebra with a derivation**
  - **An algebra is a vector space with a multiplication**
    - **A vector space over a field is a set that is closed under addition and scalar multiplication**
  - **A derivation ∂ is an operation that satisfies:**

$$\partial(a \otimes b) = (\partial a) \otimes b \oplus a \otimes (\partial b)$$

In our case:

- Field = Real numbers, r
- Set = Ordered doublets of real numbers (r_1, r_2)

${}_1D_1$ with ∂: ${}_1D_1 \rightarrow {}_1D_1$ by $\partial(r_0, r_1) = (0, r_1)$ is a Differential Algebra

How does it work? (1)

- Given the values and derivatives of two functions at the origin form (f(0) , f'(0)) and (g(0) , g'(0))
- Assume we are interested in the value and derivative of their product at the origin:

$$(f(0)g(0) , f'(0)g(0) + f(0)g'(0))$$

- This is how the product was defined in ${}_1D_1$!
- This works also for the sum of two functions

How Does It Work? (2)

- **Define the operation [ ] by**

$$[\, f(x_0) \,] = (\, f(x_0) \,,\, f'(x_0) \,)$$

- **Thus, according to the previous slide**

$$[\, f + g \,] = [\, f \,] + [\, g \,]$$
$$[\, f \cdot g \,] = [\, f \,] \cdot [\, g \,]$$

- **For any function that can be represented by finitely many additions and multiplications (this includes most common intrinsic functions available on a computer) the following holds:**

$$[\, f(x) \,] = f([x])$$

- **For a real x we have [x] = (x,1) = x + d, d = (0,1), so we can conclude that**

$$(\, f(x) \,,\, f'(x) \,) = f(x+d)$$

Advanced Applications

- $({}_1D_1, \partial)$ can be generalized into $({}_nD_v, \partial_1, \ldots, \partial_v)$ for computation of derivatives up to order n of functions in v variables
- It can be generalized to vector functions (transfer maps)
- Composition of maps: given two vector functions with known derivatives up to order n, what are the derivatives of their composition? If M(0) = 0, then

$$[\, N \circ M \,]_n = [\, N \,]_n \circ [\, M \,]_n$$

- Can be used to compute inverses $[M^{-1}]_n$

Applications in Beam Physics

Transfer Map Method and Differential Algebras

- The transfer map $\mathcal{M}$ is the flow of the system ODE.

$$\vec{z}_f = \mathcal{M}(\vec{z}_i, \vec{\delta}),$$

  where $\vec{z}_i$ and $\vec{z}_f$ are the initial and the final condition, $\vec{\delta}$ is system parameters.

- For a repetitive system, only one cell transfer map has to be computed. Thus, it is much faster than ray tracing codes (i.e. tracing each individual particle through the system).
- The Differential Algebraic method allows a very efficient computation of high order Taylor transfer maps.
- The Normal Form method can be used for analysis of nonlinear behavior.

Differential Algebras (DA)

- it works to arbitrary order, and can keep system parameters in maps.
- very transparent algorithms; effort independent of computation order.

The code **COSY Infinity** has many tools and algorithms necessary.

COSY Infinity

- Arbitrary order
- Maps depending on parameters (mass dependence!)
- No approximations in motion or field description
- Large library of elements
- Arbitrary Elements (you specify fields)
- Very flexible input language
- Powerful interactive graphics
- Errors: position, tilt, rotation
- Tracking through maps
- Normal Form Methods
- Spin dynamics
- Fast fringe field models using SYSCA approach
- Reference manual (80 pages) and Programming manual (90 pages)

Applications of COSY

- Interactive design of spectrometers
- Interactive design of accelerator lattices
- High-order analysis
- Fringe field analysis
- Measured fields
- Error analysis, parameter dependences
- Closed orbit, lattice parameters, parameter dependence of these
- Normal Form, resonant and non-resonant, resonance driving terms

Elements in COSY

- Magnetic and electric multipoles
- Superimposed multipoles
- Combined function bending magnets with curved edges
- Electrostatic deflectors
- Wien filters
- Wigglers
- Solenoids, various field configurations
- 3 tube electrostatic round lens, various configurations
- Exact fringe fields to all of the above
- Fast fringe fields (SYSCA)
- General electromagnetic element (measured data)
- Glass lenses, mirrors, prisms with arbitrary surfaces
- Misalignments: position, angle, rotation

All can be computed to arbitrary order, and the dependence on any of their parameters can be computed.

The COSY Language

- Structured Language with nesting of procedures
- Object oriented; allows direct DA and picture variables
- Flow control statements including optimization

```
BEGIN ;
   VARIABLE ;
   PROCEDURE ;     ENDPROCEDURE ;
   FUNCTION ;      ENDFUNCTION ;
      <assignments>
      <procedure calls>
      IF ;            ENDIF ;
      WHILE ;         ENDWHILE ;
      LOOP ;          ENDLOOP ;
      FIT ;           ENDFIT ;
END ;
```

Symmetry-Based Theory

Generic transfer matrix of a cell, in the usual canonical coordinates, and mass and charge as parameters.

Only midplane and time-independence symmetry is assumed.

$$\vec{z} = (x, a, y, b, \delta, \delta_m, \delta_q)$$

$$M = \begin{pmatrix} (x|x) & (x|a) & 0 & 0 & (x|\delta) & (x|\delta_m) & (x|\delta_q) \\ (a|x) & (a|a) & 0 & 0 & (a|\delta) & (a|\delta_m) & (a|\delta_q) \\ 0 & 0 & (y|y) & (y|b) & 0 & 0 & 0 \\ 0 & 0 & (b|y) & (b|b) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Matrix of Reversed and Total Systems

$$M_r = \begin{pmatrix} (a|a) & (x|a) & 0 & 0 & (a|\delta)(x|a)-(a|a)(x|\delta) & (a|\delta_m)(x|a)-(a|a)(a|\delta_m) & (a|\delta_q)(x|a)-(a|a)(x|\delta_q) \\ (a|x) & (x|x) & 0 & 0 & (a|\delta)(x|x)-(a|x)(x|\delta) & (a|\delta_m)(x|x)-(a|x)(x|\delta_m) & (a|\delta_q)(x|x)-(a|x)(x|\delta_q) \\ 0 & 0 & (b|b) & (y|b) & 0 & 0 & 0 \\ 0 & 0 & (b|y) & (y|y) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

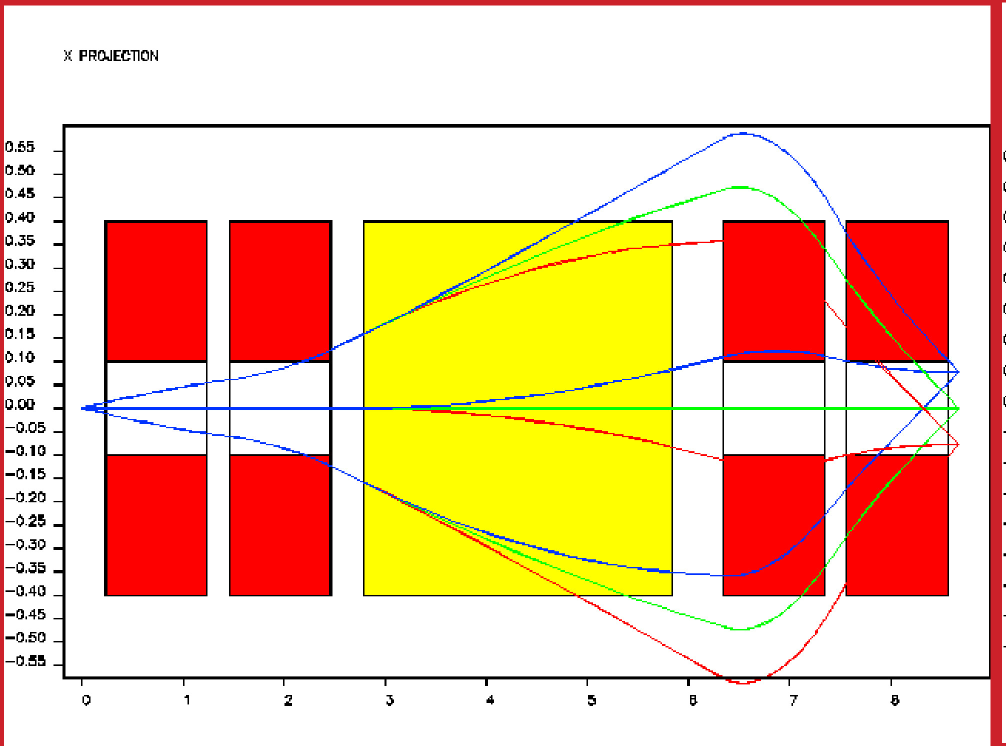
$$R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

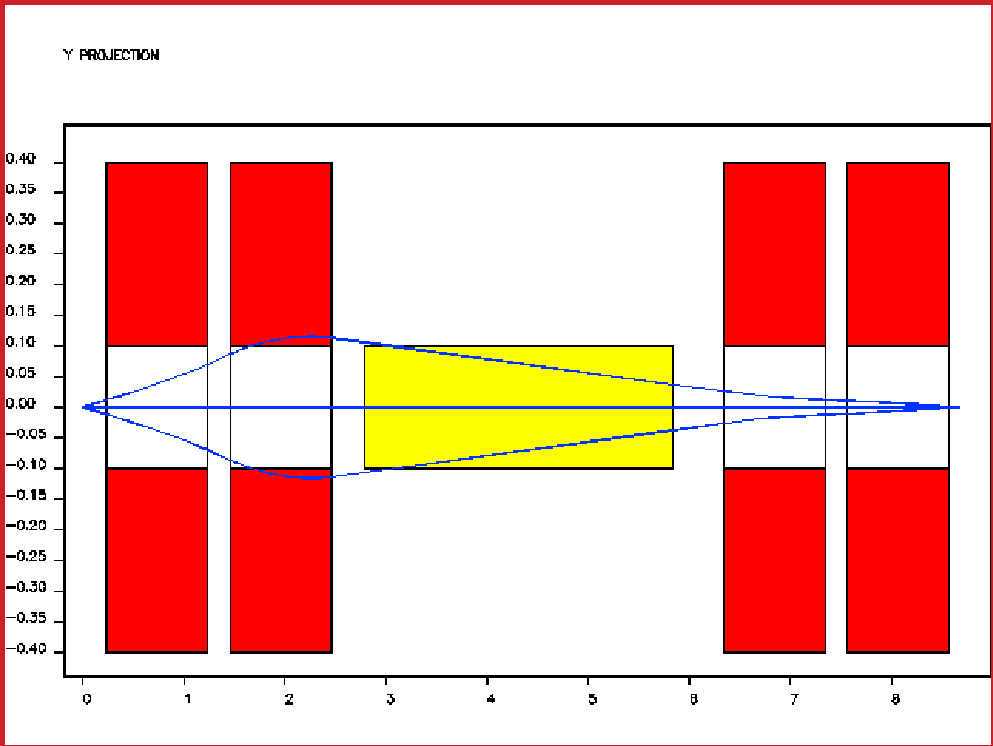
$$M_{tot} = MM_r = MRM^{-1}R$$

$$M_{tot} = MM_r = \begin{pmatrix} (x|x)(a|a)+(x|a)(a|x) & 2(x|a)(a|a) & 0 & 0 & 2(a|\delta)(x|a) & 2(a|\delta_m)(x|a) & 2(a|\delta_q)(x|a) \\ 2(x|x)(a|x) & (x|x)(a|a)+(x|a)(a|x) & 0 & 0 & 2(a|\delta)(x|x) & 2(a|\delta_m)(x|x) & 2(a|\delta_q)(x|x) \\ 0 & 0 & (y|y)(b|b)+(y|b)(b|y) & 2(y|b)(b|b) & 0 & 0 & 0 \\ 0 & 0 & 2(y|y)(b|y) & (y|y)(b|b)+(y|b)(b|y) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Possible Forward Cell Solutions (1)

Simplest (only 4 quads) non-symmetric solution

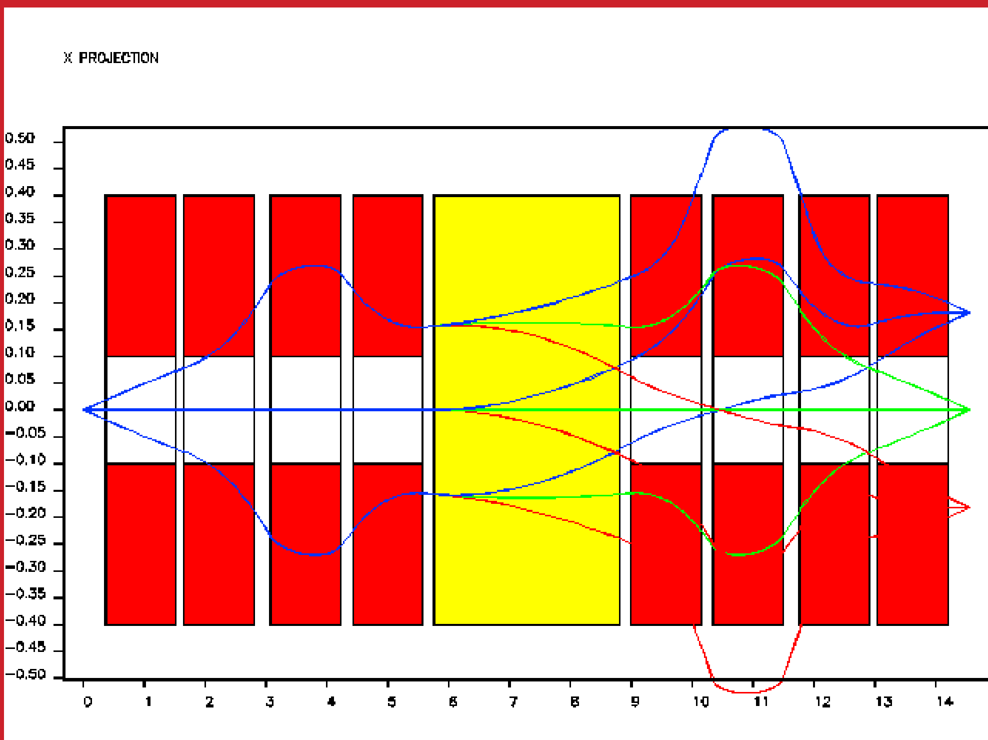


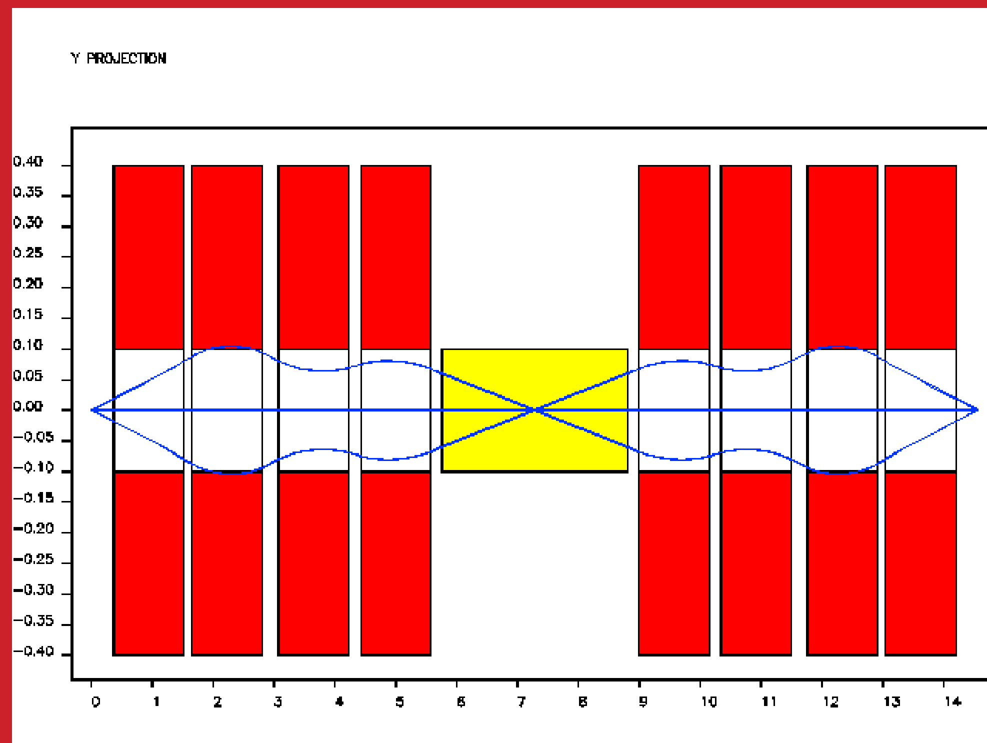


- **Advantages:** simple, good linear resolution, small intrinsic aberrations, small vertical envelope
- **Disadvantages:** large horizontal envelope, difficult to correct the aberrations

Possible Forward Cell Solutions (2)

Simple symmetric solution with intermediate vertical image

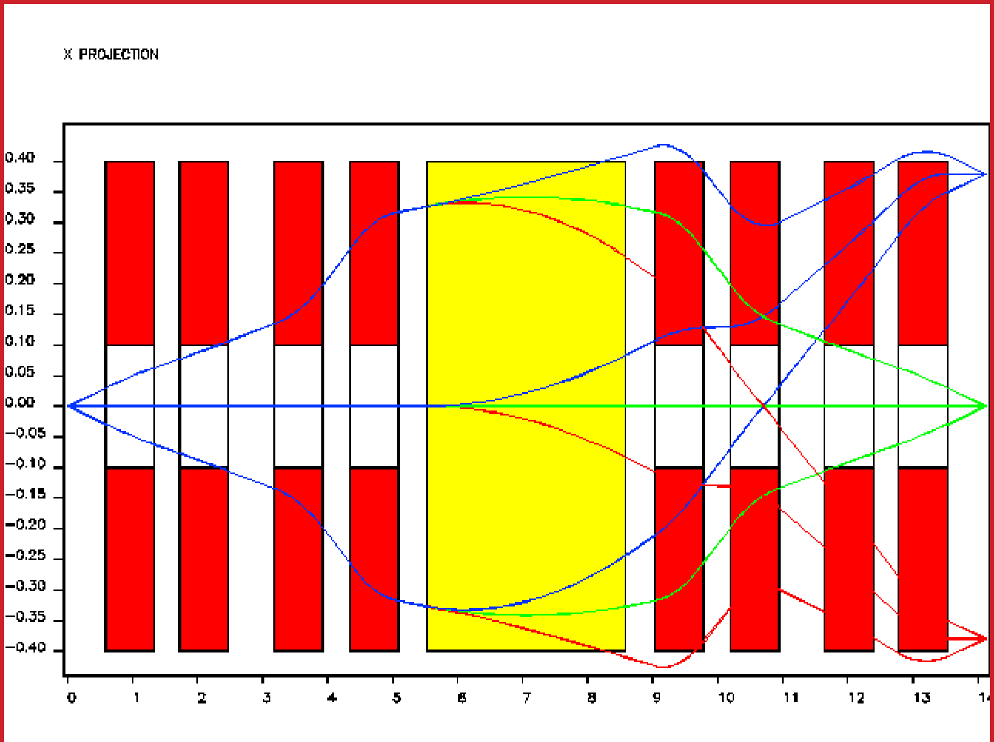


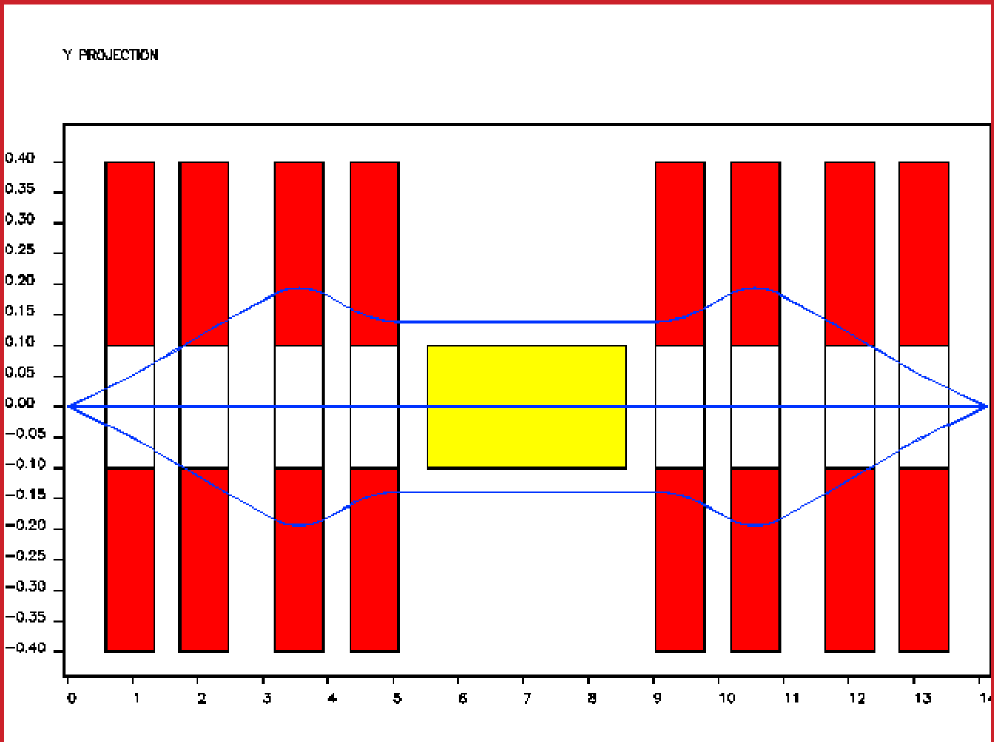


- **Advantages:** small vertical envelope
- **Disadvantages:** reduced resolution, large horizontal envelope, large aberrations

Possible Forward Cell Solutions (3)

Simple symmetric solution without intermediate images

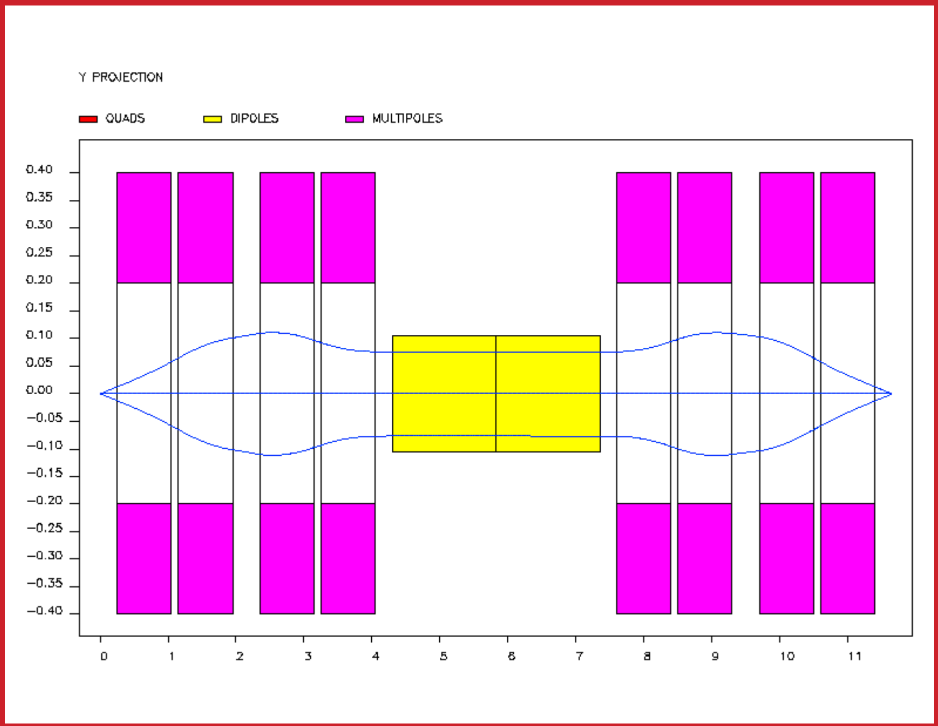




- **Advantages:** best linear resolution, intrinsic aberrations not too large, acceptable horizontal envelope
- **Disadvantages:** large vertical envelope

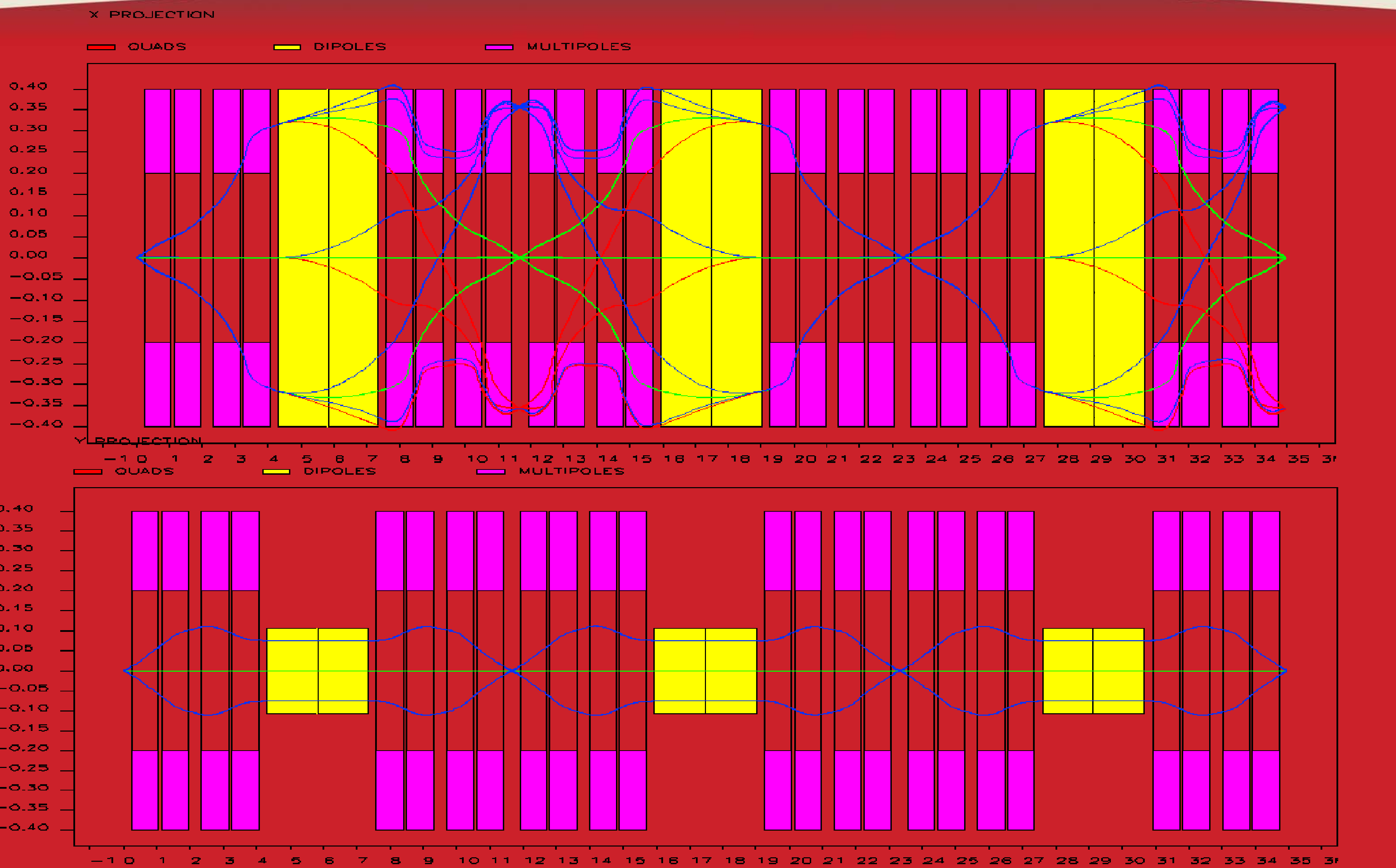
Possible Forward Cell Solutions (4)

Symmetric solution, not parallel-to-parallel vertically



- **Advantages:** good linear resolution, small horizontal and vertical envelopes
- **Disadvantages:** larger intrinsic aberrations

First Order Solution



Nonlinear Case

$$[\mathcal{M},\mathcal{R}] = \mathcal{M}\circ\mathcal{R} - \mathcal{R}\circ\mathcal{M}$$

$$\text{If } [\mathcal{M},\mathcal{R}] = 0 \;\Rightarrow\; \mathcal{M}_{tot} = \mathcal{I}$$

Map elements appearing in the commutator are:

- in **x** and **y**: all map elements that are **odd** in **a** and **b**
- in **a** and **b**: all map elements that are **even** in **a** and **b**

Map Elements of the Commutator

- (x|…)
  - **First order: (x|a)**
  - **Second order: (x|xa), (x|aδ), (x|yb)**
  - **Third order: (x|xxa), (x|xaδ), (x|xyb), (x|aaa), (x|ayy), (x|abb), (x|aδδ), (x|ybδ)**
- (a|…)
  - **First order: (a|x), (a|δ)**
  - **Second order: (a|xx), (a|xδ), (a|aa), (a|yy), (a|bb), (a|δδ)**
  - **Third order: (a|xxx), (a|xxδ), (a|xaa), (a|xyy), (a|xbb), (a|xδδ), (a|aaδ), (a|ayb), (a|yyδ), (a|bbδ), (a|δδδ)**
- (y|…)
  - **First order: (y|b)**
  - **Second order: (y|xb), (y|ay), (y|bδ)**
  - **Third order: (y|xxb), (y|xay), (y|xbδ), (y|aab), (y|ayδ), (y|yyb), (y|bbb), (y|bδδ)**
- (b|…)
  - **First order: (b|y)**
  - **Second order: (b|xy), (b|ab), (b|yδ)**
  - **Third order: (b|xxy), (b|xab), (b|xyδ), (b|aay), (b|abδ), (b|yyy), (b|ybb), (b|yδδ)**

Interrelationships Due to Symplecticity (1)

- **This allows for 9 commutator elements to be minimized by only minimizing 4.**
  - **(a|aa)~(x|xa)**
  - **(x|yb)~(b|ab)~(y|ay)**
  - **(a|bb)~(y|xb)**
  - **(a|yy)~(b|xy)**

- **These elements do not appear in the commutator:**
  - **(a|xa)~(x|xx)**
  - **(a|aδ)~(x|xδ)**
  - **(x|bb)~(y|ab)**
  - **(x|yy)~(b|ay)**
  - **(b|bδ)~(y|yδ)**
  - **(a|yb)~(b|xb)~(y|xy)**

~ means proportional

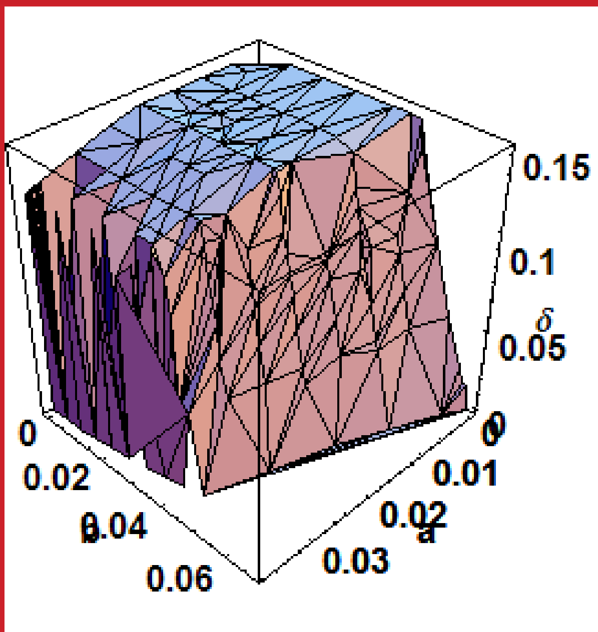
Interrelationships Due to Symplecticity (2)

- (x|xxa)~(a|xaa)
- (a|aaδ)~(x|xaδ)
- (x|xyb)~(a|ayb)~(b|xab)~(y|xay)
- (x|ayy)~(b|aay)
- (x|ybδ)~(b|abδ)~(y|ayδ)
- (a|xyy)~(b|xxy)
- (a|yyδ)~(b|xyδ)
- (a|xbb)~(y|xxb)
- (a|bbδ)~(y|xbδ)
- (x|abb)~(y|aab)
- (y|yyb)~(b|ybb)

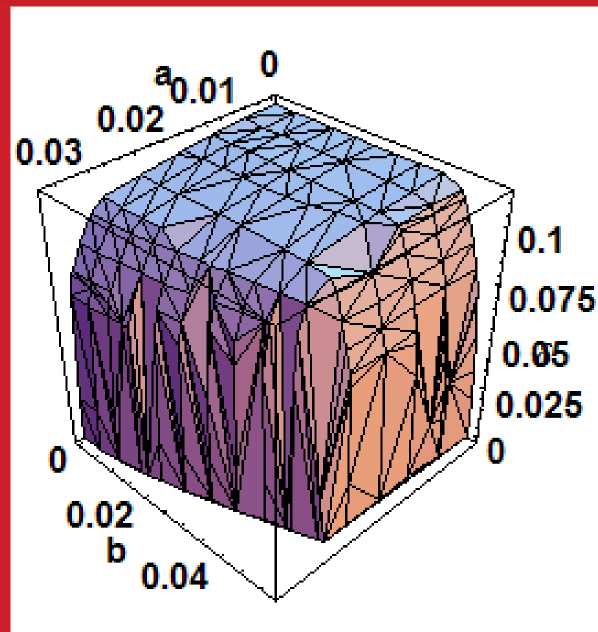
Applying all symmetry constraints it follows that if the **4 first order** conditions are satisfied, by correction of **4 second order** and **10 third order** aberrations gives a **perfect third order achromat**

Acceptance Plots – No Wedge

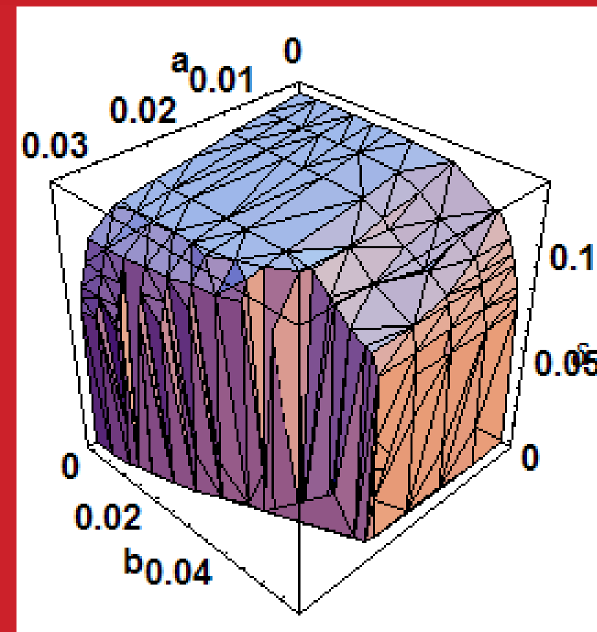
2nd order

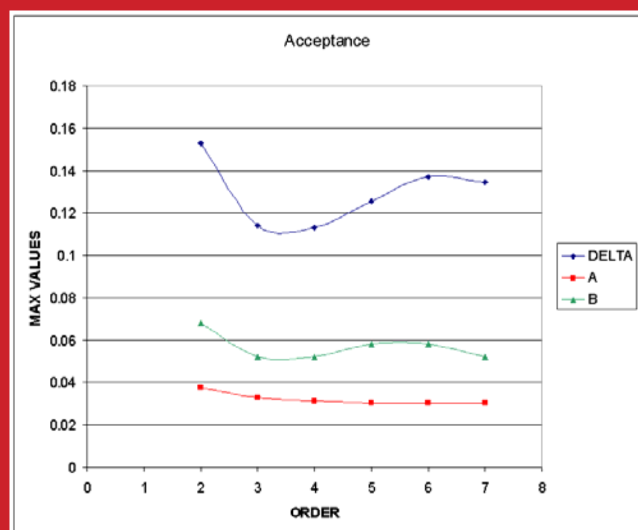


4th order



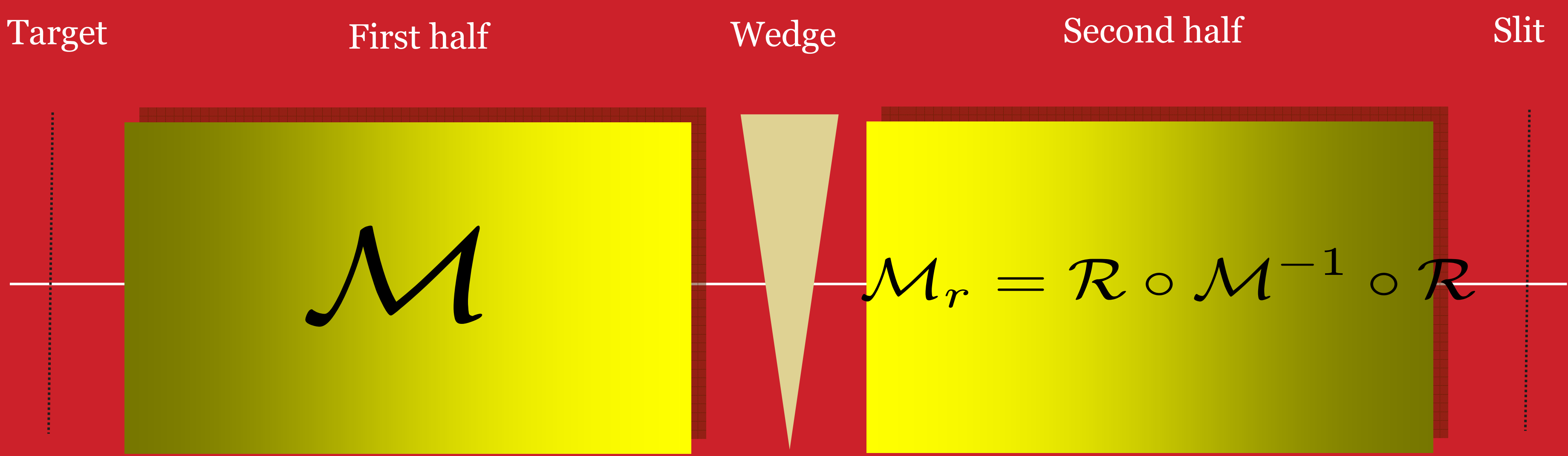
5th order





Optics of (One-Stage) Fragment Separators

Whole system mirror symmetric w.r.t the middle of the wedge



The idea is to take a high order achromat an insert the wedge such that as many symmetry properties as possible are maintained.

Moreover, some of the remaining aberrations may be eliminated by properly shaping the wedge.

Maps Involved

- Map of the wedge is a drift with a complicated energy component

$$\delta_f = (\delta|x)_w x_i + (\delta|a)_w a_i + (\delta|\delta)_w \delta_i + (\delta|xx)_w x_i^2 + (\delta|xa)_w x_i a_i + (\delta|aa)_w a_i^2$$
$$+ (\delta|x\delta)_w x_i \delta_i + (\delta|a\delta)_w a_i \delta_i + (\delta|bb)_w b_i^2 + (\delta|\delta\delta)_w \delta_i^2,$$

- Map of the separator up to the wedge (from achromat theory)

$$\begin{aligned}
x_f &= -x_i + (x|\delta)\,\delta_i + (x|xx)\,x_i^2 + (x|aa)\,a_i^2 + (x|x\delta)\,x_i\delta_i + (x|yy)\,y_i^2 + (x|bb)\,b_i^2 + (x|\delta\delta)\,\delta_i^2,\\
a_f &= -a_i + (a|xa)\,x_i a_i + (a|a\delta)\,a_i\delta_i + (a|yb)\,y_i b_i,\\
y_f &= -y_i + (y|xy)\,x_i y_i + (y|ab)\,a_i b_i + (y|y\delta)\,y_i\delta_i,\\
b_f &= -b_i + (b|xb)\,x_i b_i + (b|ay)\,a_i y_i + (y|b\delta)\,b_i\delta_i,\\
\delta_f &= \delta_i
\end{aligned}$$

- Map of the whole system

$$\mathcal{M}_{tot} = \mathcal{R} \circ \mathcal{M}^{-1} \circ \mathcal{R} \circ \mathcal{M}_d\left(-\frac{l_w}{2}\right) \circ \mathcal{M}_w \circ \mathcal{M}_d\left(-\frac{l_w}{2}\right) \circ \mathcal{M}$$

Linear Theory

- Transfer matrix of the whole system

$$\begin{pmatrix} 1-(x|\delta)(\delta|x)_w & (x|\delta)\left[\frac{l_w}{2}(\delta|x)_w-(\delta|a)_w\right] & 0 & 0 & (x|\delta)\left[(x|\delta)(\delta|x)_w+(\delta|\delta)_w-1\right] \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -(\delta|x)_w & \frac{l_w}{2}(\delta|x)_w-(\delta|a)_w & 0 & 0 & (x|\delta)(\delta|x)_w+(\delta|\delta)_w \end{pmatrix}$$

=0

=0

Conditions imposed

Main linear effect of the wedge is to increase the magnification (beside introducing mass and charge dispersions)

$$\begin{pmatrix} (\delta|\delta)_w & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -(\delta|x)_w & 0 & 0 & 0 & 1 \end{pmatrix}$$

Second Order Analytic Theory (1)

The second order part of $\mathcal{M}_{tot}$ is complicated. However, under the linear constraints and $x_i, y_i \to 0$ the results simplify to

$$
\begin{aligned}
x_f &=_2 (x|aa)_{tot}\, a_i^2 + (x|a\delta)_{tot}\, a_i\delta_i + (x|bb)_{tot}\, b_i^2 + (x|\delta\delta)_{tot}\, \delta_i^2, \\
a_f &=_2 0, \\
y_f &=_2 0, \\
b_f &=_2 0, \\
\delta_f &=_2 (\delta|aa)_{tot}\, a_i^2 + (\delta|a\delta)_{tot}\, a_i\delta_i + (\delta|bb)_{tot}\, b_i^2 + (\delta|\delta\delta)_{tot}\, \delta_i^2,
\end{aligned}
$$

where the x_f elements in the total map are

$$
\begin{aligned}
(x|aa)_{tot} &= (x|aa)\left[1 - (\delta|\delta)_w\right] - \frac{l_w^2}{4}(\delta|xx)_w\,(x|\delta) + \frac{l_w}{2}(\delta|xa)_w\,(x|\delta) + (\delta|aa)_w\,(x|\delta), \\
(x|a\delta)_{tot} &= l_w\,(\delta|xx)_w\,(x|\delta)^2 - (\delta|xa)_w\,(x|\delta)^2 + \frac{l_w}{2}(\delta|x\delta)_w\,(x|\delta) - (\delta|a\delta)_w\,(x|\delta), \\
(x|bb)_{tot} &= (x|bb)\left[1 - (\delta|\delta)\right] + (\delta|bb)_w\,(x|\delta), \\
(x|\delta\delta)_{tot} &= (x|\delta\delta)\left[1 - (\delta|\delta)\right] + (\delta|xx)_w\,(x|\delta)^3 + (\delta|x\delta)_w\,(x|\delta)^2 + (\delta|\delta\delta)_w\,(x|\delta),
\end{aligned}
$$

and similarly complicated functions for $(\delta|\ldots)_{tot}$.

Second Order Analytic Theory (2)

Using the four free knobs, the following solution eliminates all second order aberrations, including the energy aberrations of the form $(\delta|...)$:

$$(x|aa) = \frac{1}{(\delta|x)_w}\left[\frac{l_w}{4}(\delta|xa)_w + \frac{l_w^2}{8\,(x|\delta)}(\delta|x\delta)_w - \frac{l_w}{4\,(x|\delta)}(\delta|a\delta)_w - (\delta|aa)_w\right],$$

$$(x|bb) = -\frac{(\delta|bb)_w}{(\delta|x)_w},$$

$$(x|\delta\delta) = \frac{1}{(\delta|x)_w}\left[\frac{(x|\delta)^2}{l_w}(\delta|xa)_w - \frac{(x|\delta)}{2}(\delta|x\delta)_w - \frac{(x|\delta)}{l_w}(\delta|a\delta)_w - (\delta|\delta\delta)_w\right],$$

$$(\delta|xx) = \frac{(\delta|xa)_w}{l_w} - \frac{(\delta|x\delta)_w}{2\,(x|\delta)} + \frac{(\delta|a\delta)_w}{l_w\,(x|\delta)}.$$

Best practical alternative: since $(x|a\delta)$ is always small anyway, just fit $(x|aa)$, $(x|bb)$ and wedge curvature to cancel $(x|aa)_{tot}$, $(x|bb)_{tot}$ and $(x|\delta\delta)_{tot}$. This requires 2 additional sextupoles per cell or neglecting a couple of angular aberrations!

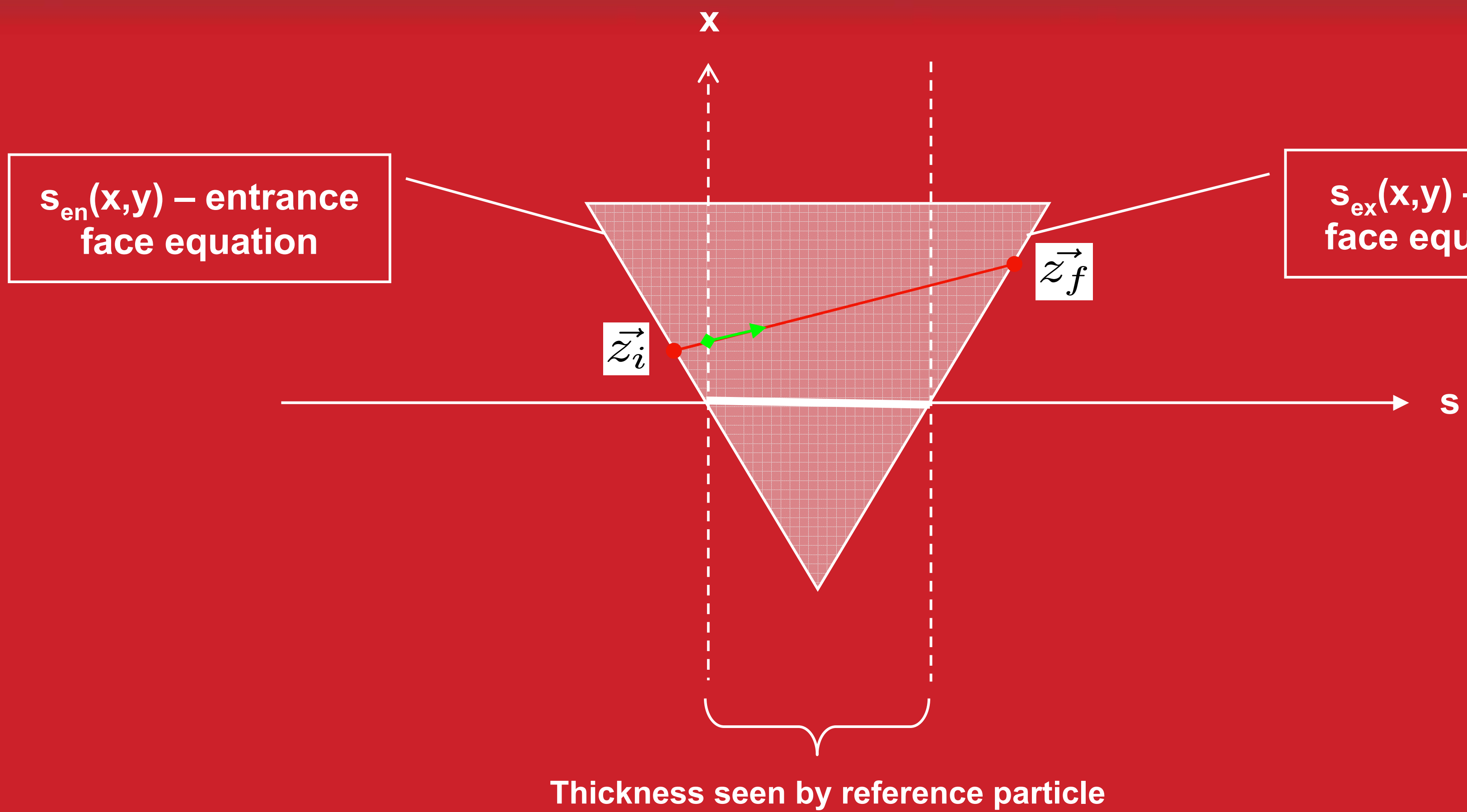
Arbitrary Order Numerical Procedure

- **Algorithm for the map of the absorber:**
  - Entrance and exit shapes regarded as curved surfaces
  - Project particle trajectories onto these sections
  - Compute the distance between them in DA
  - Solve the following equation in DA for the final energy dispersion (use DA inversion)

$$Range(E_i) - [Thickness(\vec{z_i}) + Range(E_f)] = 0$$

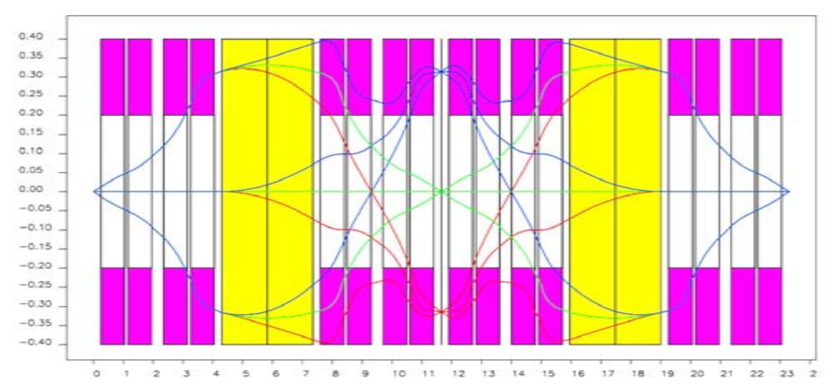
  - Using the distance result and the solution of the above equation compute Transport map
  - Apply coordinate transformation to canonical COSY coordinates

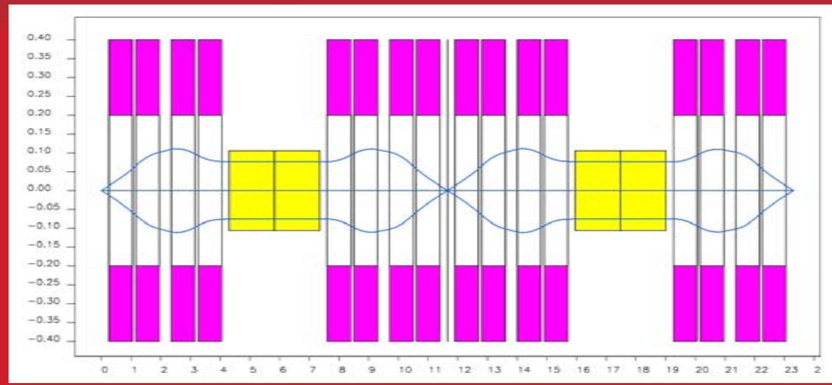
Thickness as a DA variable



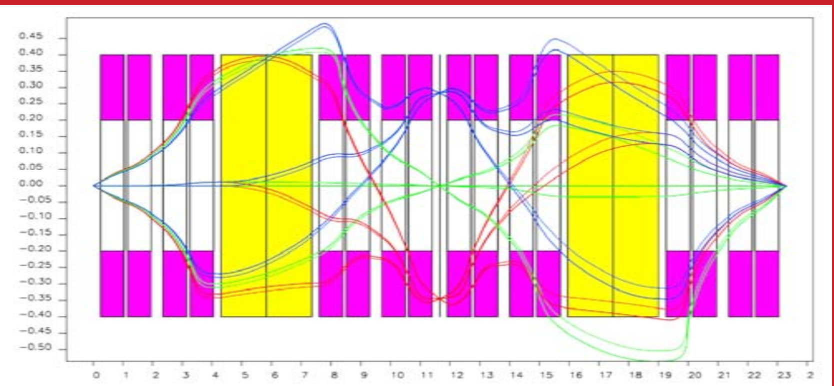
Thickness seen by any other particle is the length of the red line: computed in DA by knowing the equation of the line, the thickness seen by the reference particle, and the equations of the entrance and exit faces of the absorber

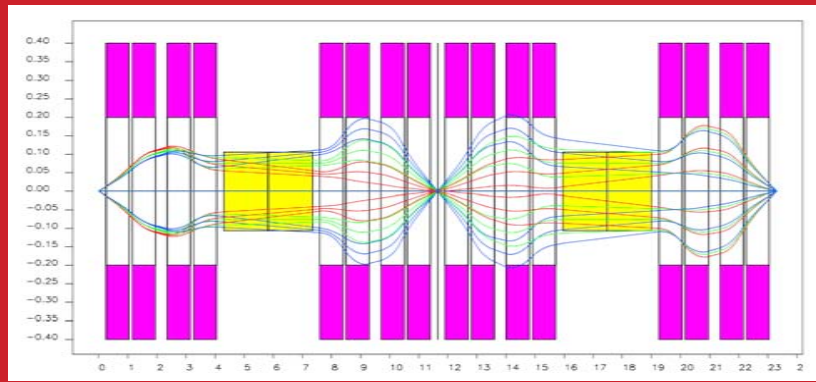
Preliminary Design



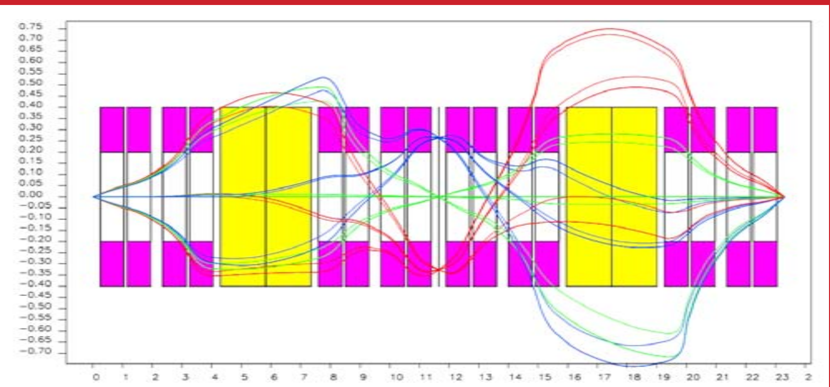


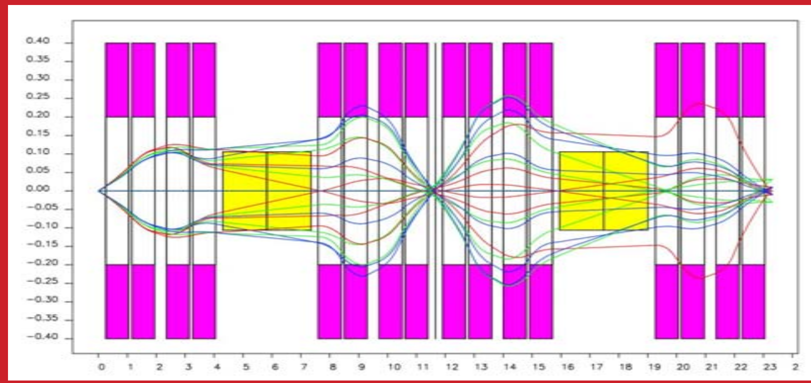
First Order





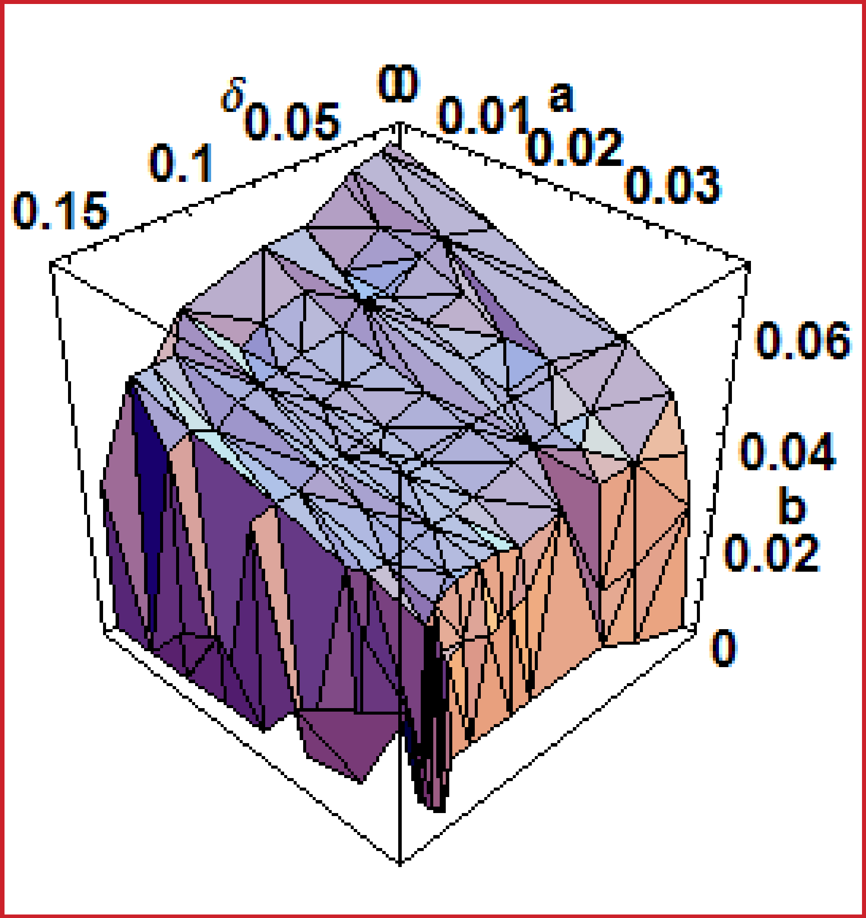
Second Order



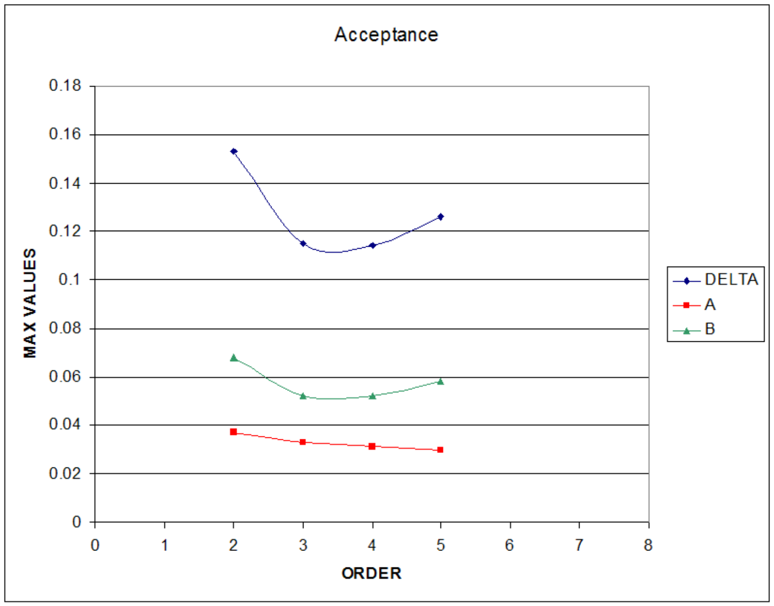


Third Order

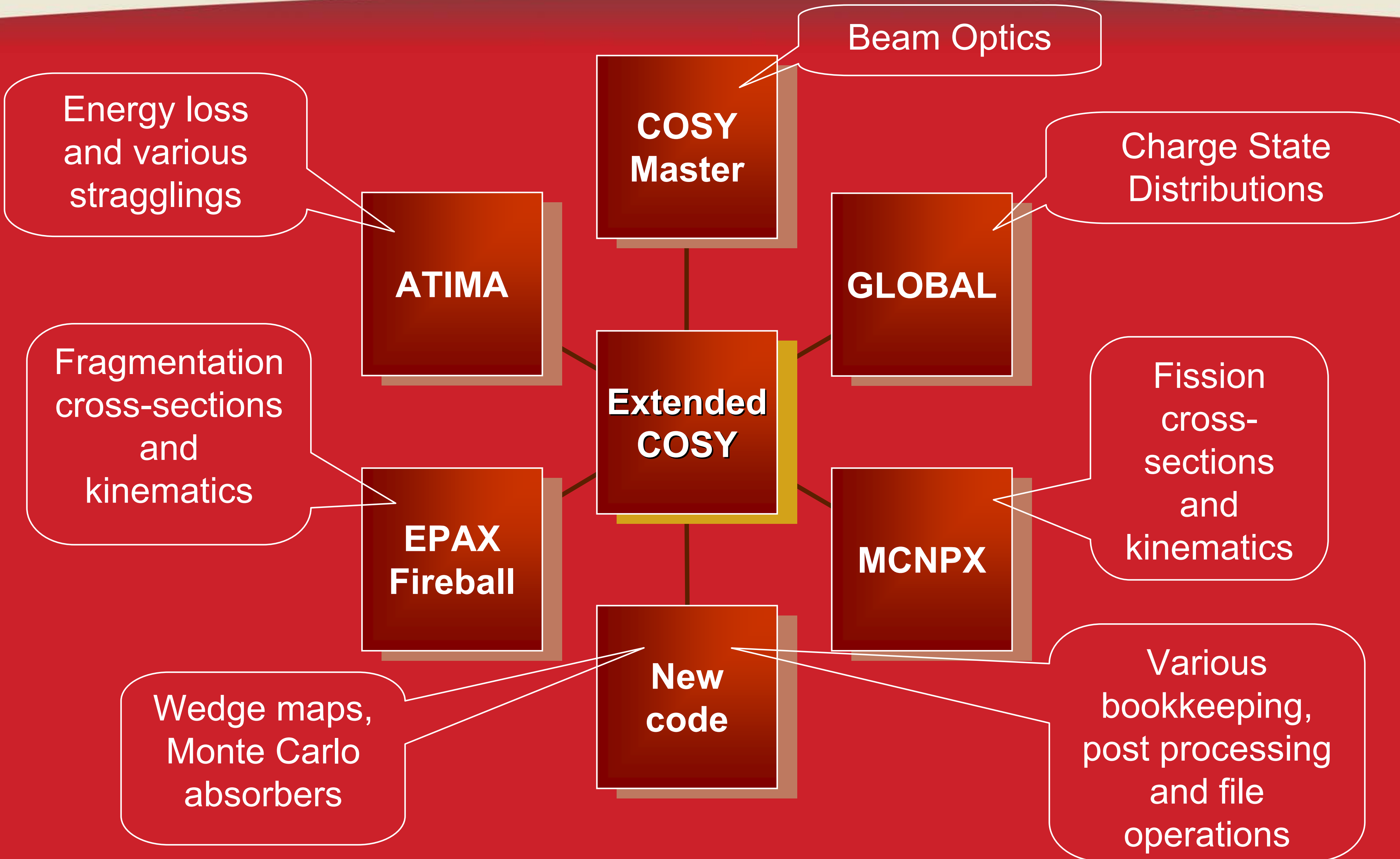
5TH ORDER ACCEPTANCE PLOTS – WITH WEDGE



Wedge thickness = 30% of range



COSY Infinity and Extensions



Extension Variants

Extended COSY

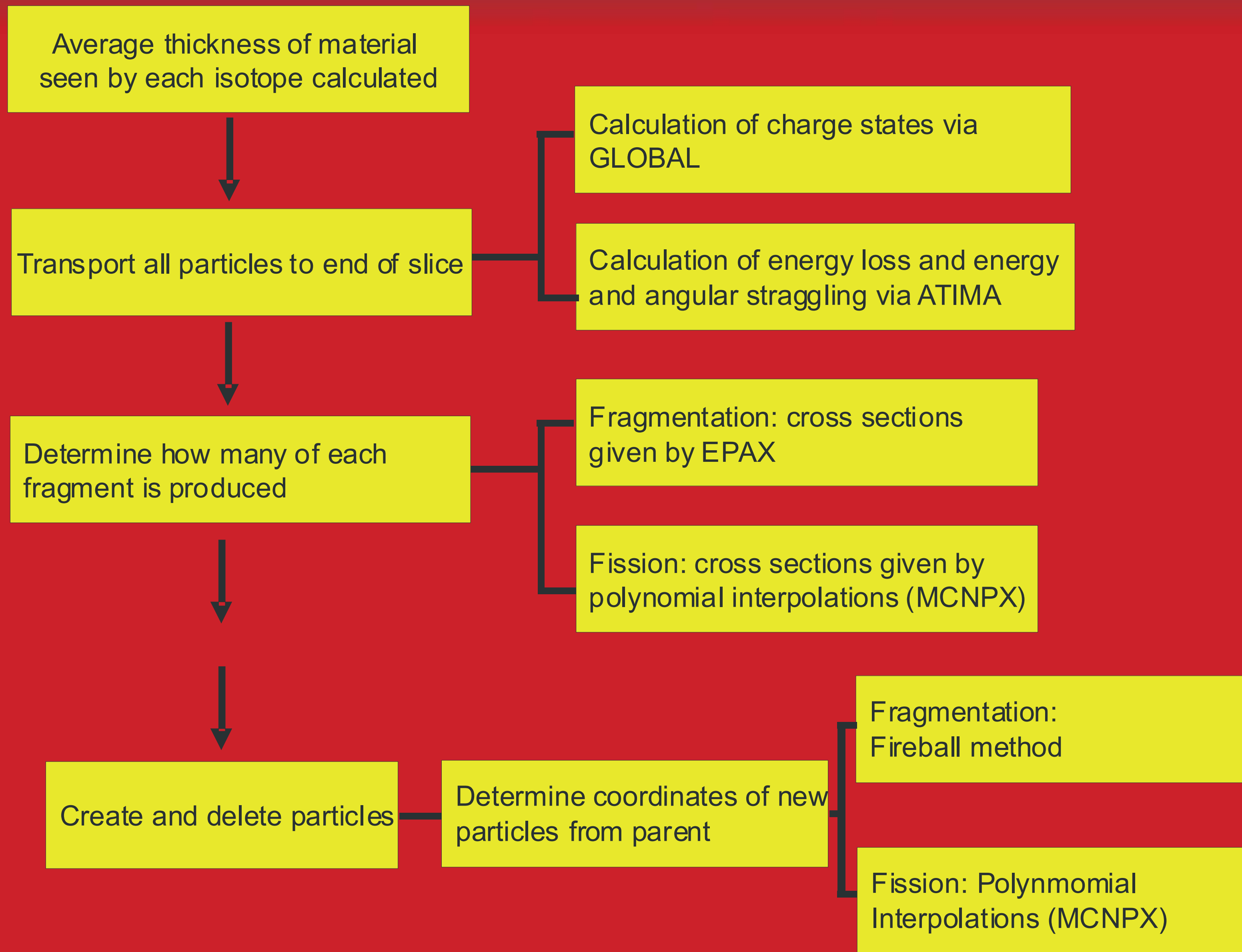
Run in Map Mode

- Fast
- Optimization is also fast
- Can be used in the design phase
- Many effects can be studied this way
- But not every aspect can be included in the maps

Run in hybrid Map-Monte Carlo Mode

- Most complete and accurate simulation
- Needed for:
  - reactions and losses in materials
  - charge exchange
  - background distribution
  - **separation purity**
- ***Optimization takes too long***

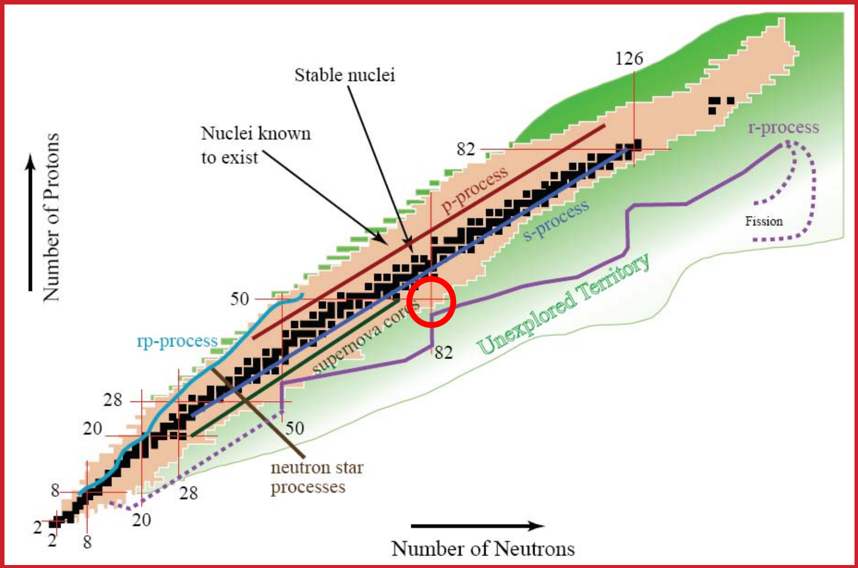
Monte Carlo Code Development
Code Flow Chart



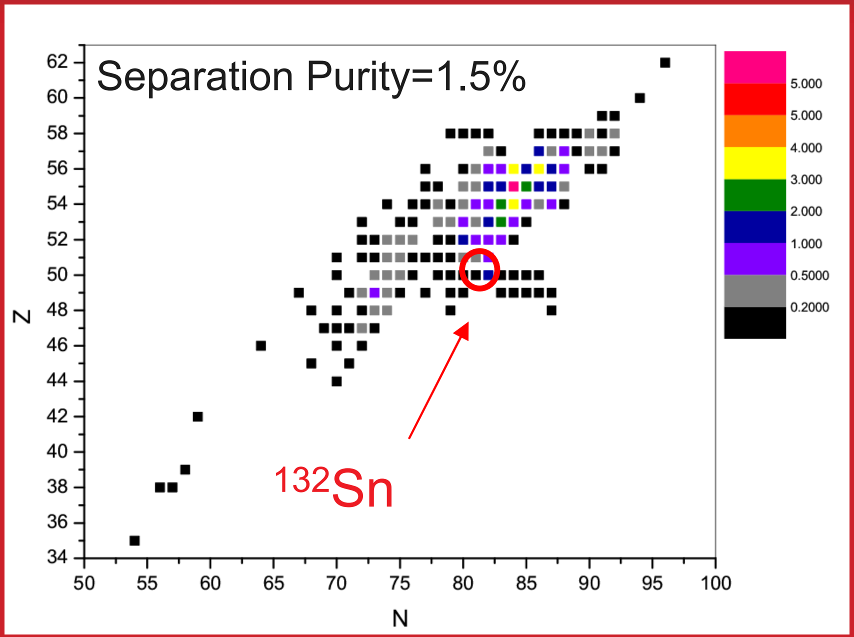
Transmission of Other Isotopes as a Function of Production Mechanism

Production Mechanism	Isotope	Transmission (%)
Light Fragmentation	^{14}Be	90.6
Heavy Fragmentation	^{100}Sn	91.0
Light Fission	^{78}Ni	21.5
Heavy Fission	^{132}Sn	42.9

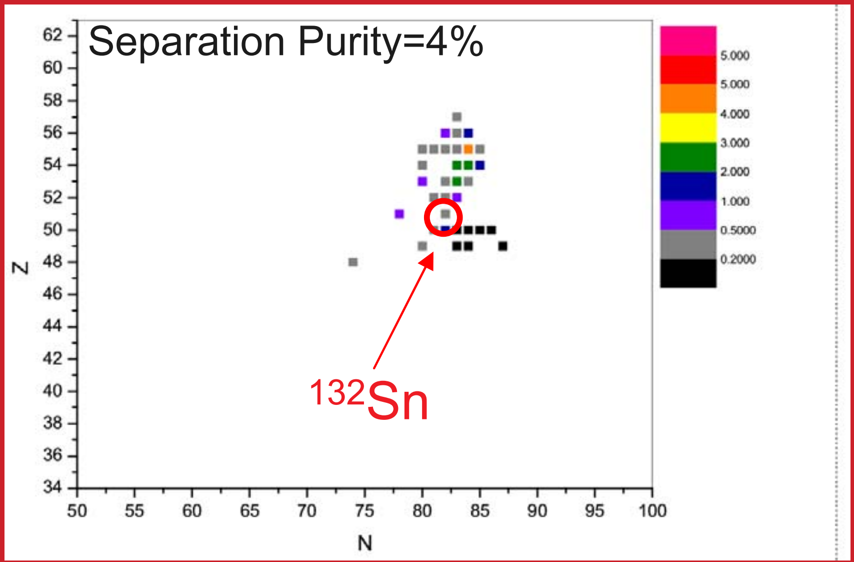
Separation Purity ^{132}Sn



First Stage →

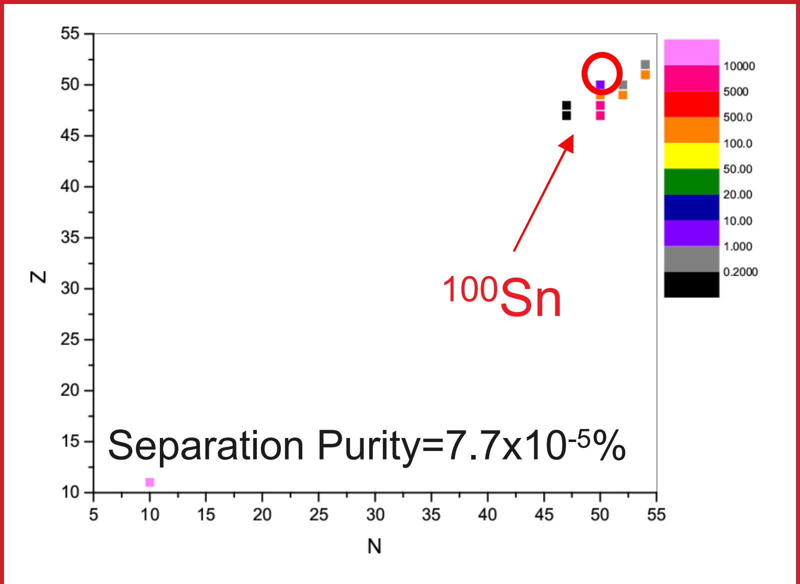


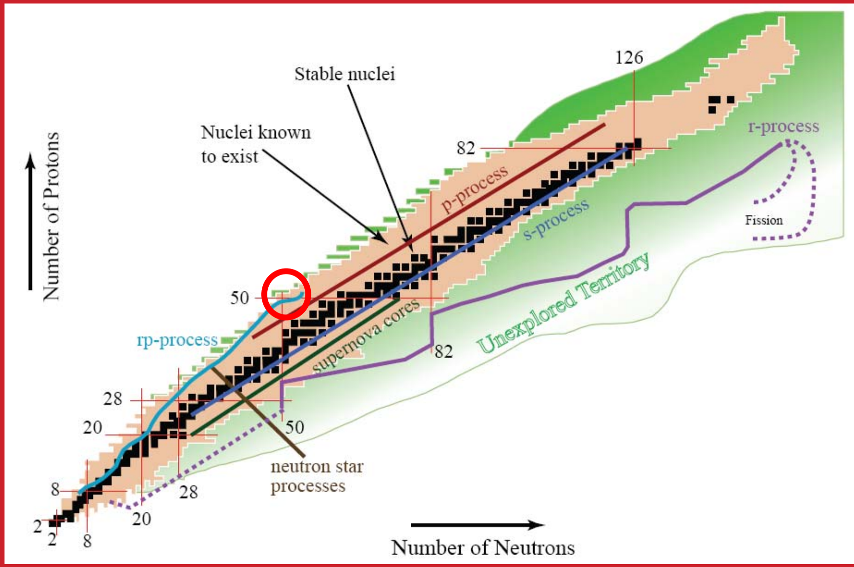
Second Stage →



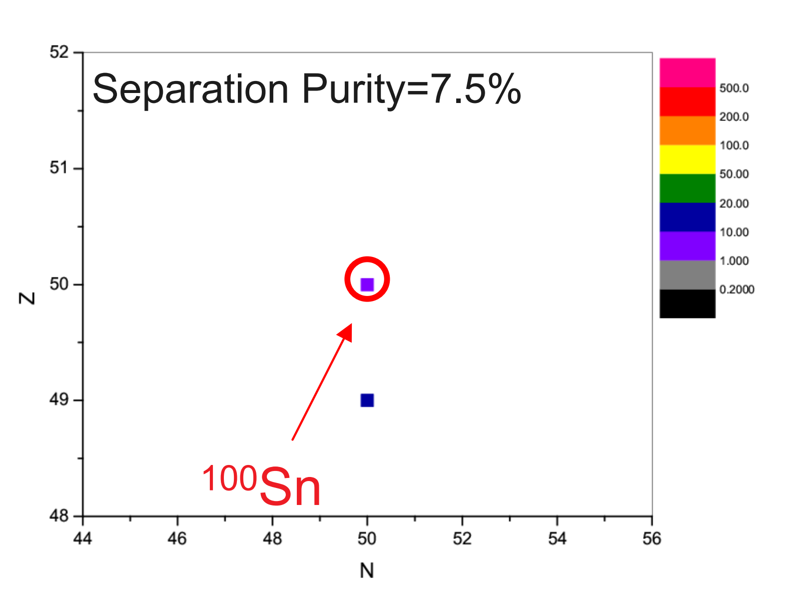
Separation Purity ^{100}Sn

First Stage →





Second Stage →



Separation Purity of Various Isotopes

Production Mechanism	Isotope	First Stage Separation Purity (%)	Second Stage Separation Purity (%)
Light Fragmentation	^{14}Be	100	
Heavy Fragmentation	^{100}Sn	7.73×10^{-5}	7.5
Light Fission	^{78}Ni	2.79×1010^{-4}	3.64×10^{-3}
Heavy Fission	^{132}Sn	1.15	4.04
Heavy Fission	^{199}Ta	8.35×10^{-3}	10.8

Computational Challenges

- Running time 2.5 days
  - On a typical PC
  - Pushed particles by 3rd order maps in vacuum and Monte-Carlo in materials
  - 10^4 initial macro-particles representing 10^8 total primary beam particles
  - n-step reactions followed up to n=10 in the target and n=5 in the wedges
  - Artificially enhanced cross-sections in a box in the N-Z plane around ^{132}Sn
- Total dataset size at the end of the run was 20 GB

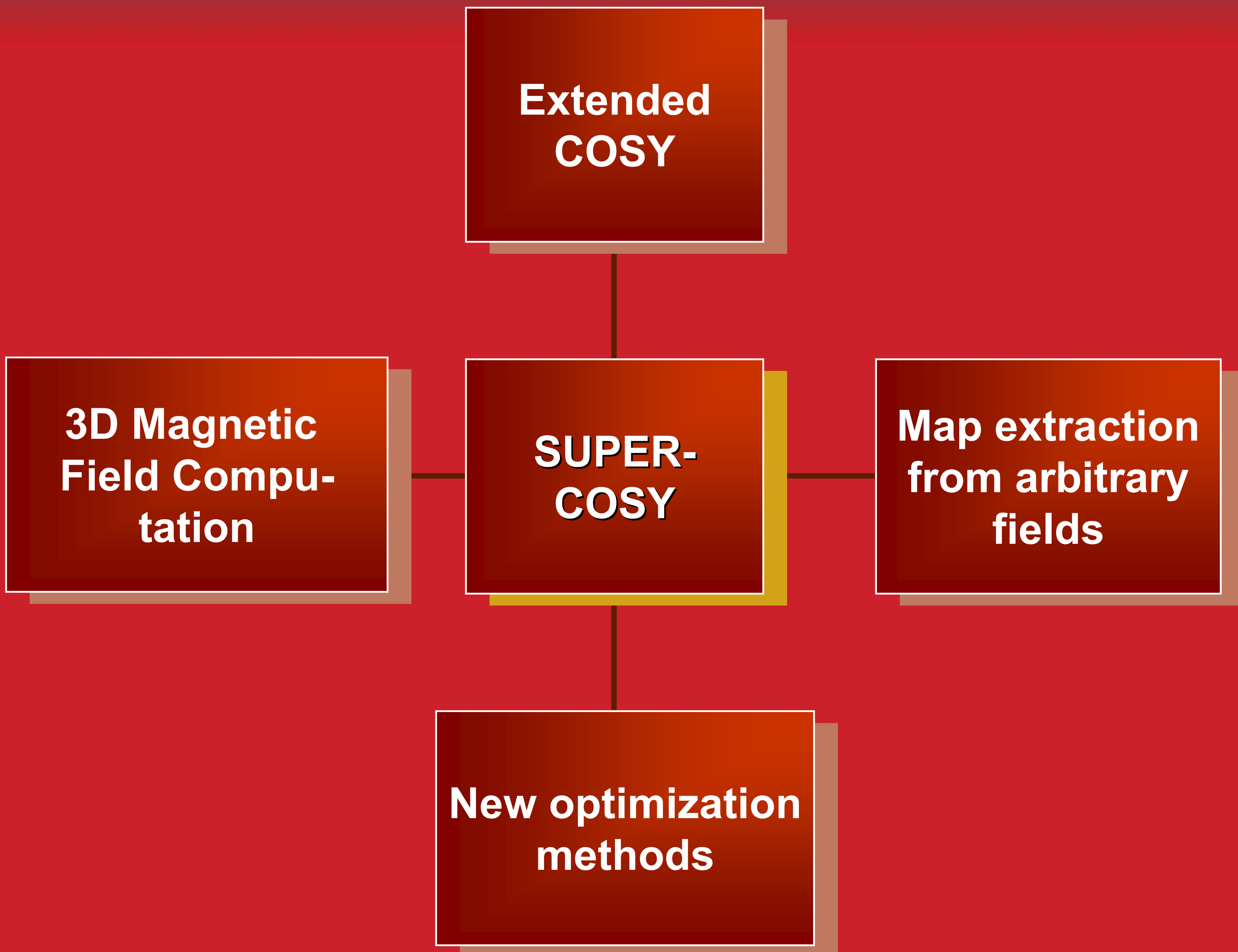
$^{124}Xe(245 MeV/u) + ^{7}Li(450 mg/cm^2) \rightarrow ^{100}Sn$

- First Stage
  - Separation Purity= 7.73 x 10^{-7}
  - Transmission= 40.5%
- Second Stage
  - Separation Purity= 7.47 %
  - Transmission= 11.6%
- Cross section ^{100}Sn= 7.12 x 10^{-9} mb
- To produce one ^{100}Sn particle in the target, 3.79 x 10^{12} primary beam particles must be used.
- Taking into account transmission losses, to have 1000 ^{100}Sn particles at the end of the second stage **3.27 x 10^{16}** primary beam particles must be used.
- DOE Grand Challenge problem, extreme scale computing

COSY in Large Scale Modeling

- **Parallelization of COSY**
  - **Stage 1 finished: MPI-based**
    - **PLOOP concept (see below)**
    - **Allows parallel single particle tracking and map-based optimization**
  - **Stage 2 in progress at MSU: OPEN-MP-based**
    - **Parallelization of COSY's low level DA tools**
    - **Potentially more powerful, but less simple and robust**
- **The PLOOP Concept**
  - **A new loop that, instead of being executed sequentially, is executed in parallel if the environment happens to be parallel**
  - **Syntax:**
    - » PLOOP **<Processor number> <Lower> <Upper>**
    - » ENDPLOOP **<Array>**

SUPER-COSY



Extended COSY
3D Magnetic Field Compu-tation
SUPER-COSY
Map extraction from arbitrary fields
New optimization methods

Summary

- **Rare isotopes are of great current interest** in nuclear physics for pure and applied science applications
- There are **facilities currently operating, under construction and planned** that are interested in experiments with rare isotope beams
- Designing, modeling, and improving rare **isotope separators require high fidelity simulations**
- We developed **an integrated beam optics-nuclear processes framework** in COSY Infinity to address this need
- **Designed** preliminary versions of **high quality separators** based on *transfer maps, DA methods and several symmetries*
- **Applied it to** a preliminary version of **FRIB** with very good results
- **Work continuing** towards:
  - Enhancing modeling, optimization and large scale computing capabilities
  - Applications to the MSU FRIB and other facilities