

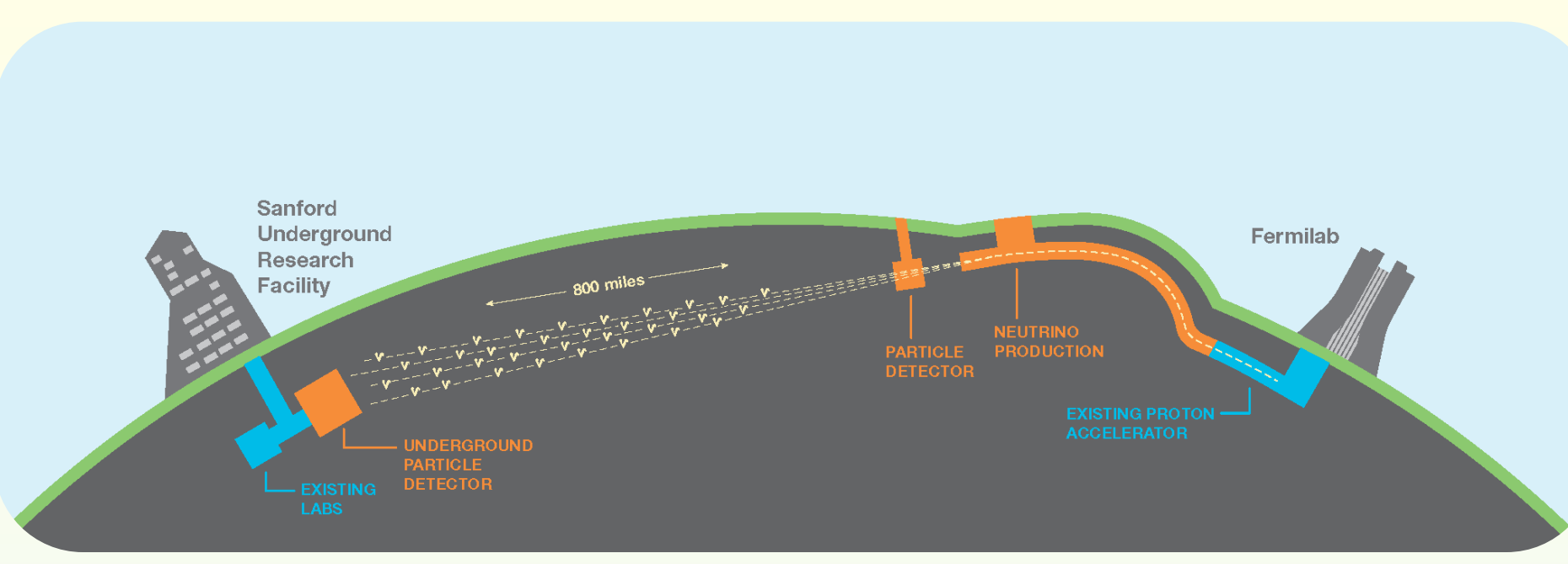
# The Community Project for Accelerator Science and Simulation 4: Advancing Accelerator Physics through High-performance Computing

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ComPASS4

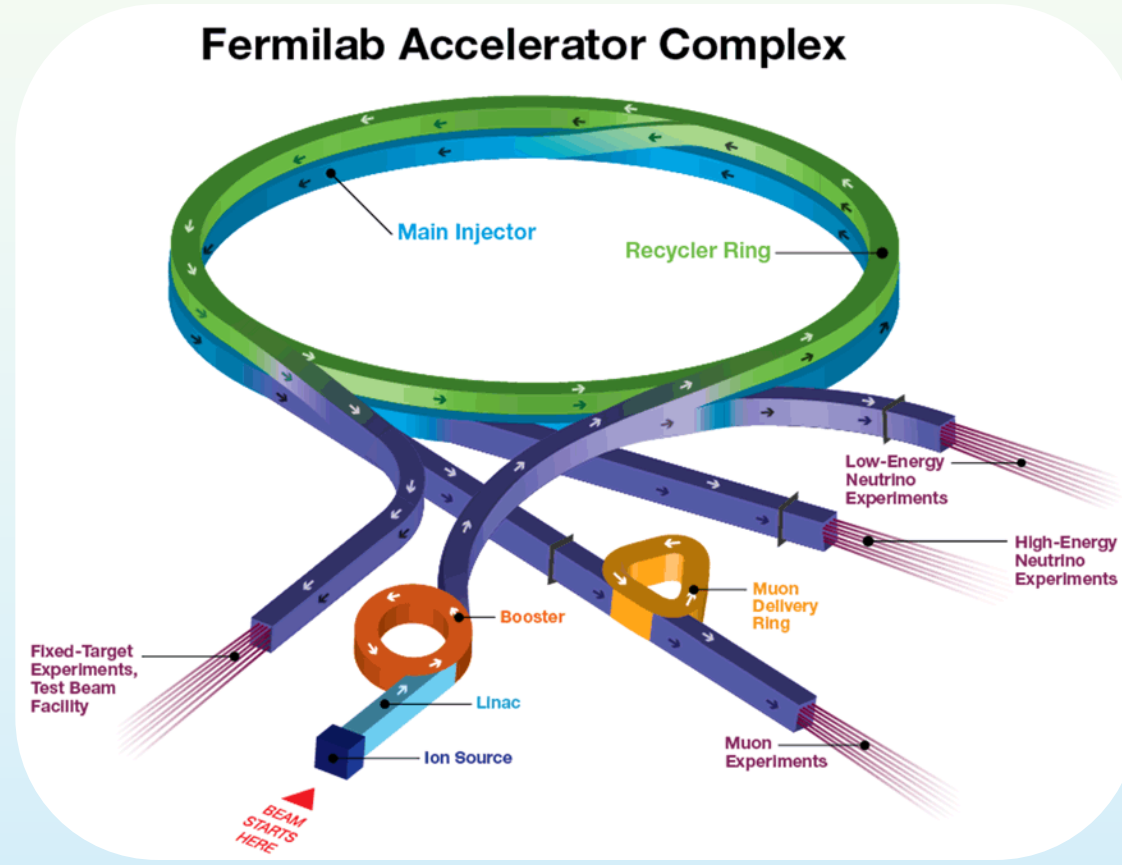
ComPASS4

## HEP Physics Drivers for Beam Dynamics



- The US High Energy Physics program is centered on high intensity physics
- The Deep Underground Neutrino Experiment (DUNE) will be the flagship experiment in the US program

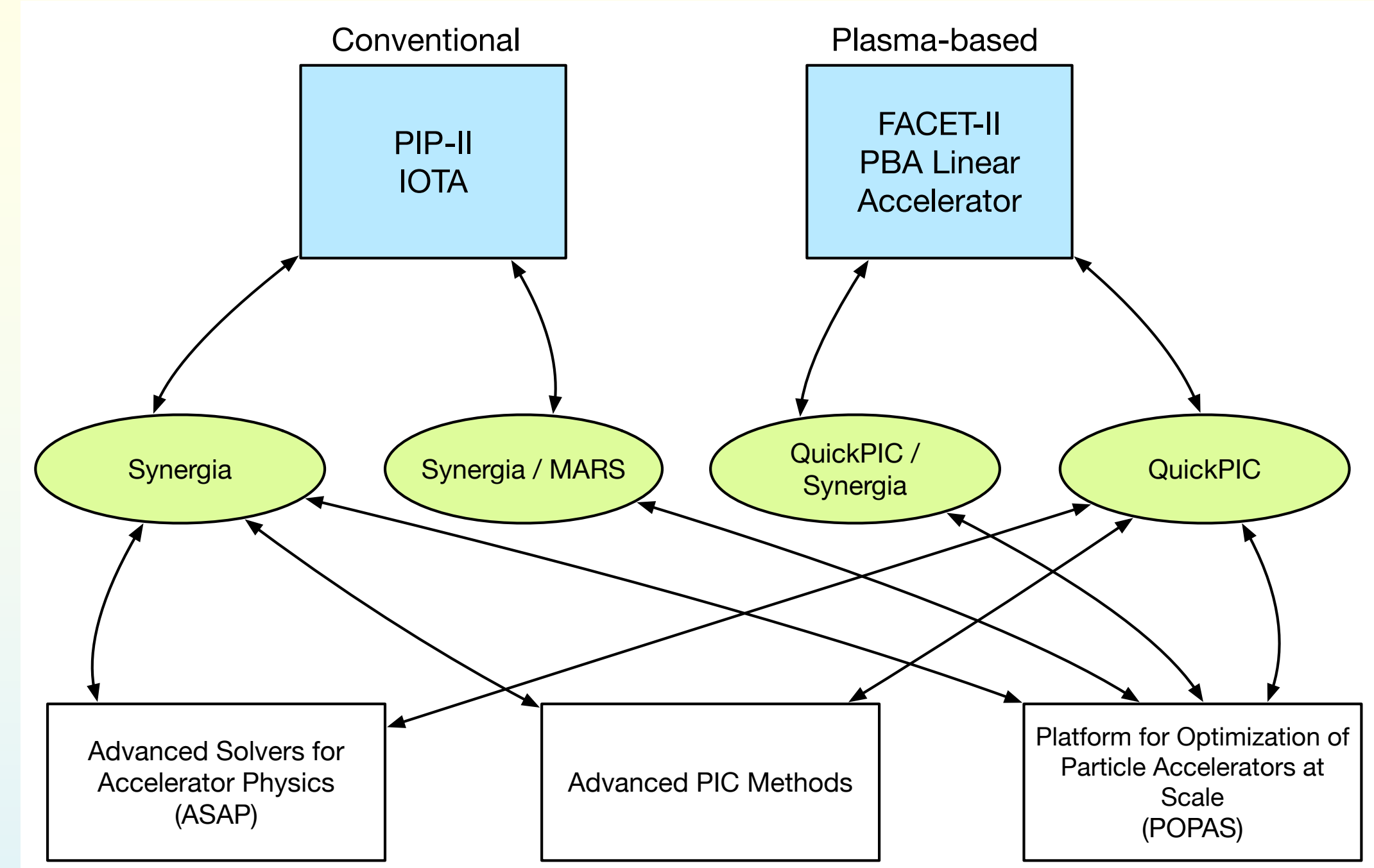
- The PIP-II project will increase the intensity of the beams produced by the Fermilab accelerator complex
  - High-intensity beams are necessary for the success of DUNE
- Simulations of intensity-dependent beam dynamics are a critical part of the PIP-II design and implementation process
- ComPASS4 is enabling and performing intensity-dependent simulations for PIP-II



- The mission of the Fermilab Accelerator Science and Technology (FAST) facility is to develop a fully-equipped R&D accelerator chain intended to support research and development of accelerator technology for the next generation of particle accelerators
- The primary focus of this effort is the Integrable Optics Test Accelerator (IOTA) ring
- ComPASS4 simulations are part of the FAST/IOTA program

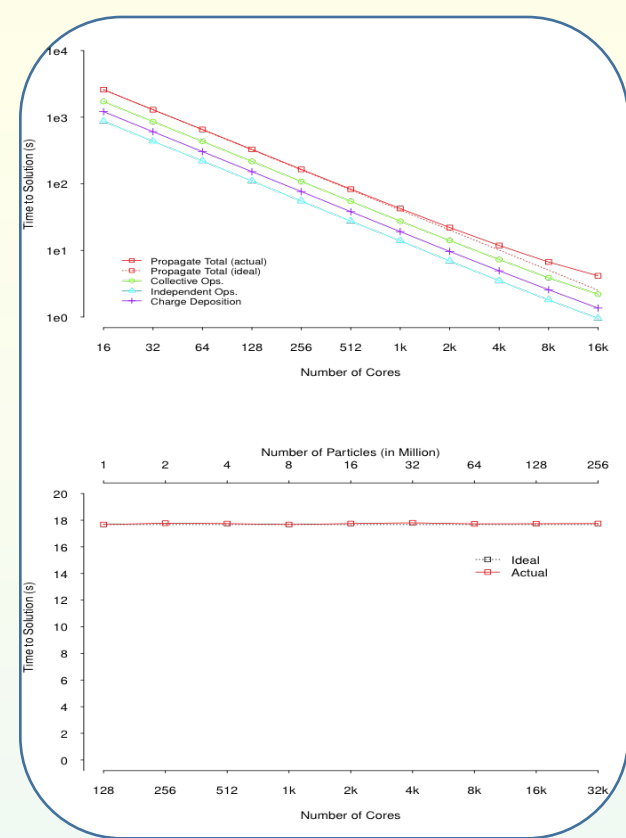
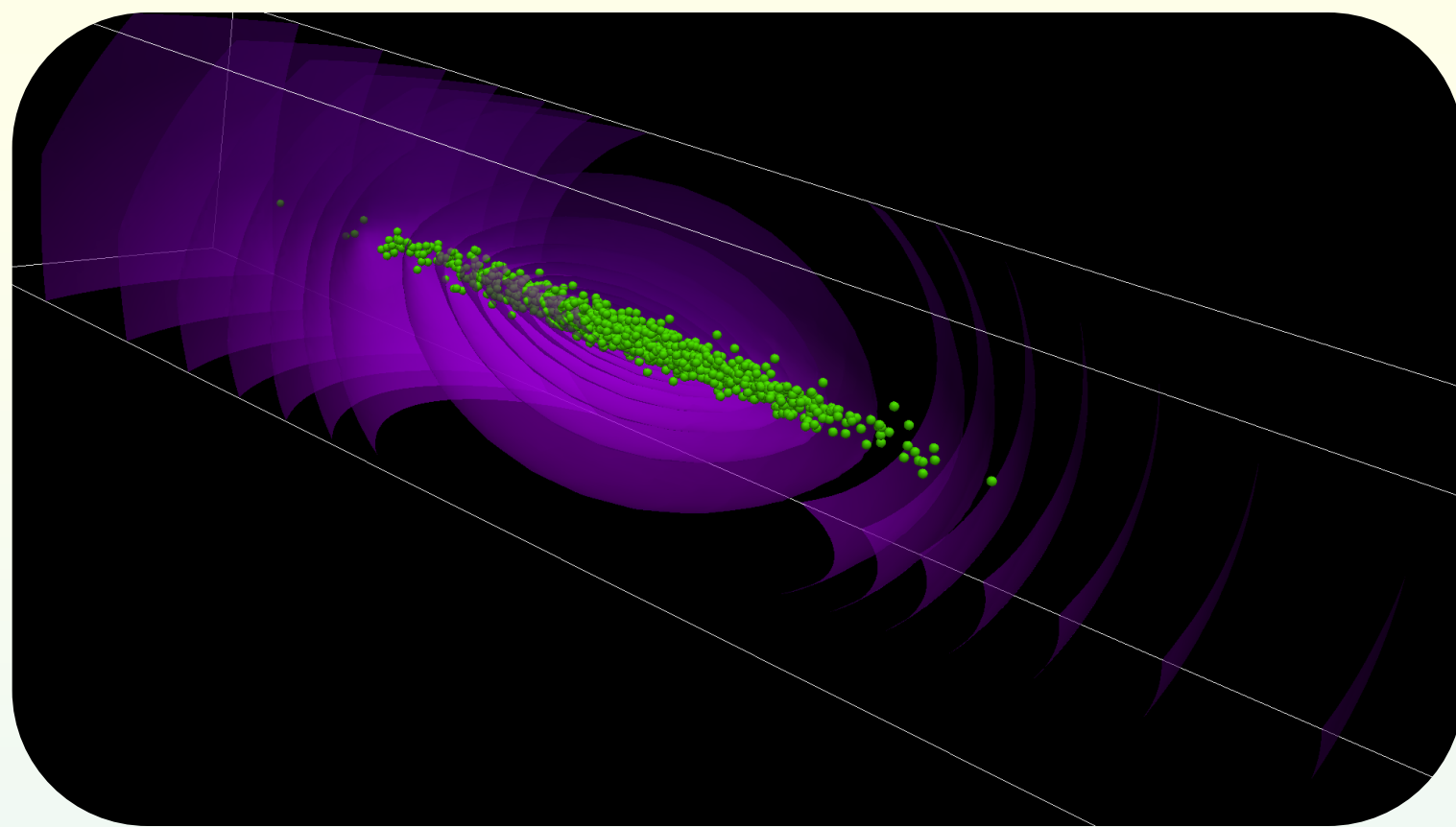


## HEP/ASCR Relationships



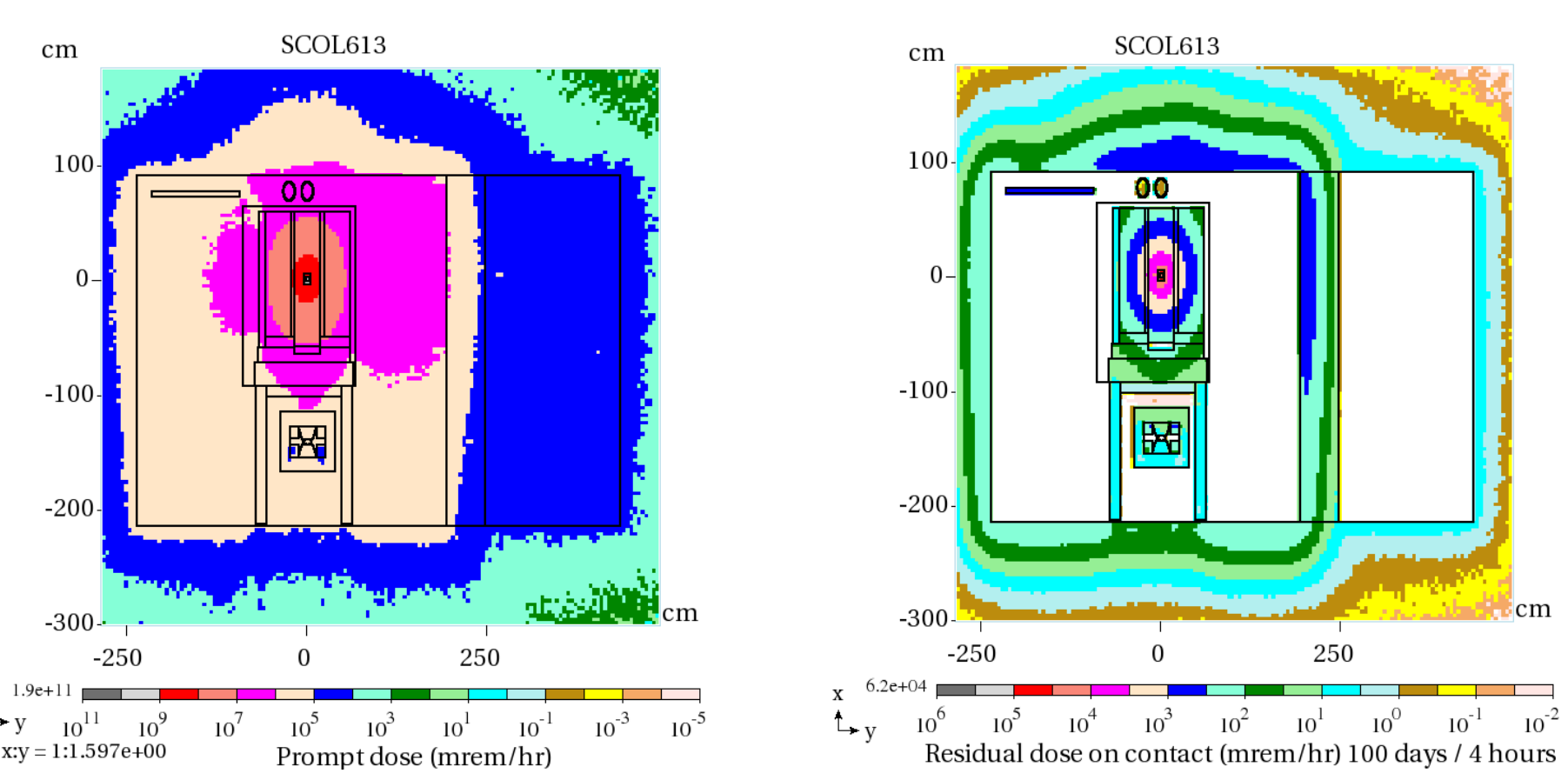
- ComPASS4 is supporting the US HEP program through the conventional accelerator programs PIP-II and IOTA as well as plasma-based experiment at FACET-II
  - Synergia and Synergia/MARS for beam dynamics
  - QuickPIC for plasma-based acceleration
- ComPASS4 accelerator physics efforts are partnering with ASCR projects in three areas
  - Advanced Solvers for Accelerator Physics (ASAP) are taking advantage of developments in linear algebra and automatic mesh refinement
  - PIC methods are being refined for modern computing architectures
  - Advanced optimization methods are being made available for general accelerator problems in the Platform for Optimization of Particle Accelerators at Scale (POPAS)
- ComPASS accelerator efforts in beam dynamics and plasma-based acceleration are being combined into a single simulation capable of handling a plasma-based linear accelerator stage with beam transport

## Synergia and Synergia/MARS



- Synergia is the primary ComPASS4 package for conventional beam dynamics
  - Linear and non-linear single-particle dynamics
  - Space charge and general wakefields
  - Tracking of single bunches, bunch trains, and overlapping bunch trains
  - Strong scaling to 10k+ procs/bunch, 100k+ procs/train

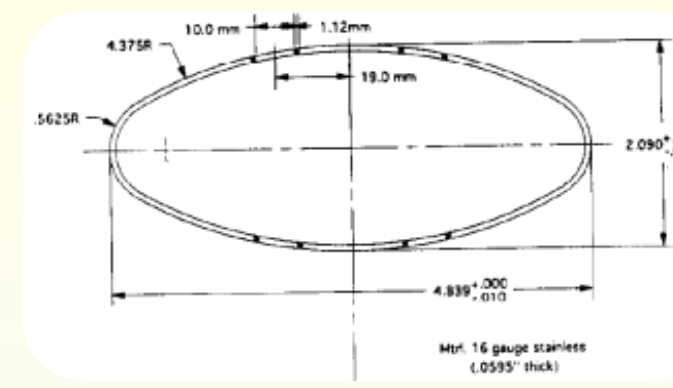
Prompt and residual dose above a particular location in the Main Injector



- Synergia/MARS is being developed as part of ComPASS4
  - MARS is a simulation package for energy deposition in matter
  - Combined Synergia/MARS will allow full simulations of beam dynamics + losses + secondary radiation
  - Includes MARS simulation of losses from Synergia as well as Synergia tracking of secondary particles from MARS

## ASAP and POPAS

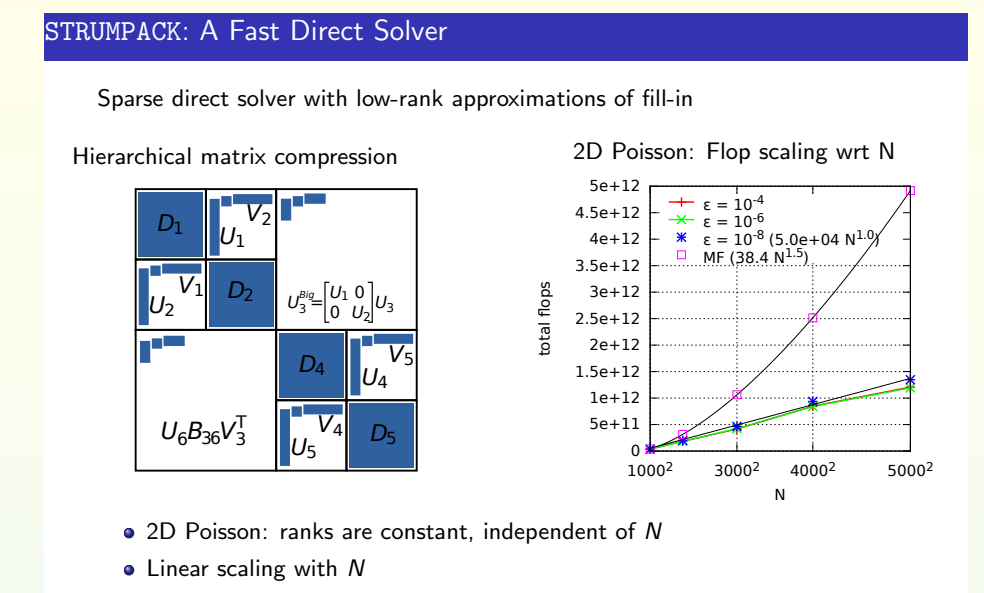
### Advanced Solvers for Accelerator Physics (ASAP)



Existing Poisson solvers in Synergia and QuickPIC use FFT-based methods

- Fast
  - Basic boundary conditions: open, rectangular
- Real machines often have non-trivial boundary conditions (left)

- ASAP will provide linear algebra-based solvers for arbitrary boundaries
- Optimized for modern architectures



### REFINEMENT WHEN DOING MULTIPLE SOLVES

- Beam dynamics
- Multiple triangular solves with different right hand sides
- No or few changes in the matrix: factorization done once
- Triangular solve done at every step
- $t_{base} = t_{ordering} + t_{matrix} + t_{fact} + N \times t_{solve}$
- $t_{refined} = t_{ordering} + t_{matrix} + t_{refine} + t_{matrix} + t_{fact} + N \times t_{solve}$
- $speedup = \frac{t_{base}}{t_{refined}}$

### Platform for Optimization of Particle Accelerators at Scale (POPAS)

POPAS is being developed as a general solution to conventional and accelerator physics optimization problems on HPC platforms

- Creating an API to handle complex parameter and objective definitions
- Take advantage of massively parallel systems
- Take advantage of automatic differentiation
  - Already present in Synergia

Optimization is the "science of better"

Find parameters (controls)  $x = (x_1, \dots, x_n)$  in domain  $\Omega$  to improve objective  $f$

$$\min_{x \in \Omega} f(x) \quad x \in \Omega \subseteq \mathbb{R}^n$$

- (Unless  $\Omega$  is very special) Need to evaluate  $f$  at many  $x$  to find a good  $x$ .
- Focus on local solutions:  $f(x_*) \leq f(x) \forall x \in \mathcal{N}(x_*) \cap \Omega$
- constraints defined the feasibility region  $\Omega$

Multiobjective Optimization

Simultaneously minimize  $n_2 > 1$  objectives

$$\min_{x \in \Omega} f_1(x), \dots, f_{n_2}(x)$$

- $f_1(x)$  dominates  $x^2$  if  $f_1(x^*) \leq f_1(x)$  for all  $x$ , and  $f_2(x^*) < f_2(x)$  for at least one  $x$ .
- $x^1$  is nondominated in  $\Omega$  if there is no  $x^2 \in \Omega$  that dominates  $x^1$ .

Formal optimal solutions: A set  $P$  of points are nondominated in  $\Omega$

- Especially useful when missing a convexity exchange between objectives
- Significantly more expensive than single-objective optimization

Why Algorithms Matter: The Accelerator Case

Varying open quadrupoles to meet beam size targets (in PELEGANT)

Heuristics often "embarrassingly naturally parallel"

- PSO: particle swarm method
- Typical through stochastic sampling/evolution
- 1024 function evaluations per iteration
- Simplex: Nelder-Mead; trust-region; is model-based trust-region algorithms
- one function evaluation per iteration

Algorithmic Differentiation

Computational Graph

- $y = \sin(x + y) + c$
- Forward and reverse modes
- AD tool provides code for your derivatives

Write codes and formulate problems with AD in mind!