Beam physics and project goals

Scientific Mission of DOE-GARD ABP to address four grand challenges:
1. **Intensity**: How do we increase beam intensities by orders of magnitude?
2. **Quality**: How do we increase beam phase-space density by orders of magnitude, beyond the current state of the art, up to the realization of virtual twins of particle accelerators, enabling design and modeling of particle accelerators at unprecedented speed, levels of accuracy, and realism; and apply these tools to key accelerator facilities relevant to DOE HEP (such as PIP-II/DUNE, FACET-II).
3. **Prediction**: How do we develop predictive “virtual particle accelerators”?

**SciDAC-5 goals**: Deliver particle accelerator and beam simulations tools that go beyond the current state of the art, up to the realization of virtual twins of particle accelerators, enabling design and modeling of particle accelerators at unprecedented speed, levels of accuracy, and realism; and apply these tools to key accelerator facilities relevant to DOE HEP (such as PIP-II/DUNE, FACET-II).

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**Computational challenges**
- Large particle number and grid resolution for high fidelity
- Support for realistic elements (3D field maps) and geometries
- Simulate beam dynamics processes on long time scales
- Exchange of data between codes in open and documented formats
- Exploit advances in computational capabilities (modern GPUs)
- Exploiting reduced models for fast optimization

**Codes and methods**

**ImpactX**
- Next generation of the code IMPACT-Z
- S-based tracking with 3D space charge
- Adaptive mesh refinement (built on AMReX)
- Parallelism with GPU acceleration
- To model beam transport in the PIP-II linac

**SciDAC Development**
- Support for RF cavity elements using realistic fields
- Magnetic elements with soft-edge fringe fields
- Lattice translation/parsers (TraceWin, MAD-X)
- Preprocessors for 3D electromagnetic field maps
- Support for openPMD particle output

**Synergia**
- Particle-in-cell based beam dynamics
- Collective effects (2.5/3-D space charge, impedance)
- Optimized for parallel operation on GPUs (but can run anywhere)
- To model injection and acceleration in the Booster

**POUNDERS**
- Efficiently optimize large-scale least-squares objectives
- Free of analytical derivatives

**SciDAC Development: Surrogate Models**
- Using machine learning to speed up simulations by orders of magnitude
- Individual calculations and segments of accelerators
- Also examining physics-informed methods

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**Optimization for Synchrotron Simulation**

The 8 GeV proton-storage Recycler Ring is essential for reaching megawatt beam intensity goals for the DUNE neutrino beam at FNAL. Custom shims on each permanent magnet were designed to cancel manufacturing defects and bring magnetic fields to the design values. Remaining imperfections cause the observed tune variation vs energy to deviate from what would be calculated from the design fields. Using the POUNDERS optimization method with Synergia in the loop, we can quickly determine values for the remnant fields which reproduce that observed variation.

The POUNDERS (“Practical Optimization Using No Derivatives for sums of Squares”) method is designed to efficiently optimize large-scale least-squares objectives when analytical derivatives are not available or difficult to compute. POUNDERS is a trust-region method that maintains internal models of the simulation outputs around the current iterate. By maintaining such models, POUNDERS often finds high-quality solutions in far fewer simulation evaluations than methods that do not exploit a sum-of-squares structure.

POUNDERS adjusted additive offsets to the sextupole and octupole moments of all shim plates collectively, seeking to minimize the squared errors with respect to chromaticity scan data from the physical machine. Our experiments yielded better than order of magnitude sum-squared-error improvements, converging on nearly the same parameter values as a simplex method. Adding higher order terms improves the convergence speed advantage over simplex, as expected. The resulting changes to the lattice parameters are under study by machine experts at Fermilab.