(WG2) Modeling and simulation tools (including energy deposition); fundamental theory and applied math. [Summary: work in progress]

Theme 1: Analytical methods. (summary by Tim Zolkin)

Analytical properties of nonlinear dynamics in accelerators are far from completely understood. We have to develop more advanced tools in order to meet future (and modern) requirements on beam brightness and quality. Two major directions are the use of analytical methods to develop conceptually new machines and tools to optimize or analyze existing accelerators.

Research topics in Theme 1:

Search of new integrable systems

- There is no general method on finding integrable conditions for dynamical systems with many degrees of freedom. Usually, we discover one by luck or by introducing sufficient symmetries. We should continue to search and possibly implement them. Examples include round beams, IOTA, use of electron lenses.
- We have to try new directions as well. We can move from integrable to near integrable, perhaps chaotic but bounded (for example systems with attractors), or even structurally stable analytical models.

General theory

- Development of perturbation techniques for quick estimates of dynamical aperture and dynamical variables such as fundamental frequencies is the direction in which we must proceed.
- We should develop a new modern language for description of nonlinear optical functions in the machine.

Incorporation of AI

- Use of AI for search of integrable systems presents two possible directions of work: (1) recognition of integrable or near-integrable systems as well as (2) development of algorithms directly searching for one.
- Use of AI for tuning or optimizing an existing lattice (or help in design of future machines) is different from using AI for operational optimization. In this case, analytical models should be used as a system to optimize.

Theme 2: Modeling of intense beams. (summary by XiaoBiao Huang)

Despite recent progress in understanding halo formation and mitigation in intense beams, there remain many unaddressed fundamental questions, such as if halo-free beam equilibria exist, if it is possible to inject beam without creating halos, and if it is possible to generate beams that can be injected without halos. Substantial development is needed in the modeling of intense beams in order to answer these questions.

The exploitation of nonlinear elements for Landau damping (e.g. HL-LHC, IOTA, PIP-III) calls for more accurate and efficient tracking algorithms in highly nonlinear or poorly characterized fields.

Numeric noise in space charge simulation could drive unphysical diffusion, which leads to incorrect prediction of beam behavior in lattices based on integrable optics. Understanding and controlling such effects would be important.

Coherent synchrotron radiation (CSR) in intense, short electron beams can severely limit the beam quality. While there have been a number of codes that implements 1D, 2D, or 2.5D models, there is currently no code that can accurately and reliably model 3D CSR effects.

In response to the above needs, the following research topics are proposed.

Research topics in Theme 2:

Modeling of Intense Beams

- Characterization of nonlinear applied fields using realistic Maxwellian models and using it for symplectic tracking
    - Algorithm to extract a concise, smooth representation of vector potential from boundary data for highly nonlinear elements (without Taylor expansion) to use in symplectic tracking of a realistic ring.
- Self-consistent matching of intense beams to a nonlinear lattice and studying the sensitivity to the initial phase space distribution
    - Extend existing recent work on beam equilibria in nonlinear lattices to the case of intense beams in a general nonlinear, s-periodic lattice to produce a numerical tool for generation of matched beams.
    - Explore other methods of generating integrable lattices and study the robustness of such lattices

- Understanding numerical particle noise in intense beams and its role in driving diffusion in nonlinear lattices and mitigating such effects
    - Apply techniques from statistical mechanics and kinetic theory to study properties of a near-integrable, nonlinear N-body Hamiltonian system of simulation particles.
    - Improved smoothing and symplectic integration reduce noise
- Design the transport for the injection into a ring (IOTA) that results in matched beams (including the effect of a kicker) or the generation of a matchable beam
    - Design a transport to match a given beam, if possible
    - If not, design a beam that can be matched to the lattice
    - Adjoint methods and machine learning could be used.
- 3D full PIC simulation for intense beams
    - Computation power has made it feasible
    - Scale disparities and boundaries
    - Symplectic, high-order PICs
    - Computation algorithms on GPUs
    - High-accuracy solvers

3D CSR Theory and Simulation Code

- Developing a 3D CSR theory that describes the full physics involved in the phenomenon.
    - w/ shielding from vacuum chamber
    - time domain or frequency domain
- Developing a 3D simulation code that can accurately and efficiently model the physical process, including transient effects, for extremely bright electron beams in accelerators.
    - Quasi-realistic vacuum chamber
    - Arbitrary phase space distribution
    - Self-consistency
    - Ability to handle ultra-short (e.g., sub-micron) bunches
    - Fast turn-around

Theme 3: Numerical tools, collaborative frameworks, virtual accelerator. (summary by Jean-Luc Vay)

No major accelerator project proceeds that hasn't been thoroughly modeled by comprehensive, detailed simulations.

There is a need for fast, reduced to full physics 6-D models (often Particle-In-Cell). Nobody seems to be able to predict halo or emittance growth even within a factor of two.

There are many beam and accelerator codes in existence, developed independently, with licenses ranging from fully open to fully closed source.

Simulations often address part of the accelerator and beam physics, sometimes missing important couplings of effects, as well as opportunities that only full system modeling offer for optimization and maximum benefits from machine learning.

There is thus the needs for:

➔ Pushing further in algorithmic and High-Performance Computing.

➔ Collaborative frameworks that run on desktop computers, supercomputers, in the cloud.

➔ Integrated, multi-physics, self-consistent, start-to-end simulations that can predict the behavior of beams in accelerators "as designed/built".

➔ For all these tasks, explore how it can use or help use **machine learning**.

Research topics in Theme 3:

Numerical tools

- High performance parallel computing is essential to predict halo and emittance growth accurately. We are not there yet ➔ need to push for faster, more accurate algorithms and codes.
- Computing hardware and technology is undergoing a generational change (e.g., CPU to GPU). Simulation programs must be upgraded to efficiently execute on new platforms.
    - Question to the community: is Fortran legacy an asset or a drawback?
- Operating systems, compilers, computing hardware, programming languages and availability of people fluent in them changes over time.
    - Software must be maintained to remain viable long-term.
    - Codes have been lost because they became unmaintainable. Their capabilities have had to be re-implemented.
- Explore how machine learning can be used to have better algorithms, more accurate and faster codes.

Collaborative frameworks

- Develop collaborative framework(s) to organize code development efforts toward integrated, multi-physics, start-to-end modeling.
- To this end, standardization of output data and input scripts should be developed and adoption encouraged.
  - Essential step to enable codes coupling and uniformization of data.
  - Can also help leveraging Machine Learning capabilities.
  - openPMD standard already widely used for particles and field data from simulations and experiments.
- Build on effort to develop online framework(s) in the Cloud (e.g., Sirepo) to enable integrated, collaborative research (with computational reproducibility) and education.
- Note: mix of licensing is possible but amount and effectiveness of collaboration increases with level of openness of the various components ➔ although open source is not required, it is favored. [this topic generated a lot of discussion]

End-to-end Virtual Accelerator (EVA) – **GC#4**

- Develop *End-to-end Virtual Accelerator (EVA)* that can predict the behavior of beams in accelerators "as designed/built".
  - Like flight simulator: EVA to allow to model operation of the accelerator in "real time".
  - Can be used to develop fast virtual models of accelerators with machine learning.
- Build on framework task to connect codes and frameworks for integrated, multi-physics, self-consistent, start-to-end simulations including "everything":
  - Accurate modeling of components.
  - Collective effects (space charge, impedance, …).
  - Dynamic machine configuration.
  - Energy deposition.
  - And everything else that matters.
- Note: specialized tools are needed to model structured plasmas for next generation accelerators (MHD or Vlasov-Fokker-Planck)
  - Plasma channels for acceleration.
  - Plasma lenses for focusing.
  - Plasma afterglow diagnostics.