Beam Dynamics Optimization in High-Brightness Electron Injectors

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Overview

- Introduction and motivation
 - High brightness e beam requirements for ~MHz FEL
 - Comments on multiobjective optimization tools
- Applications to APEX and LCLS-II
 - APEX design and measurement analysis
 - LCLS-II injector design studies
- Additional developments
 - New optimization algorithms: VPES-PMDE
 - Global start-to-undulator FEL optimization
- Summary and conclusions





Introduction and motivation







High-Brightness Electron Beam Requirements for ~1 MHz Repetition Rate Soft X-Ray FEL (eg, LCLS-II)

LCLS-II Baseline (0-4 GeV)



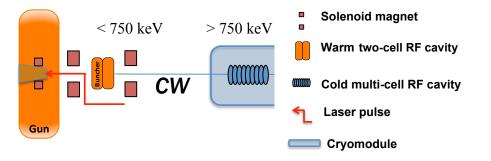
FEL Features

high repetition rate (up to 1 MHz) high average brightness (>20 W) broad photon energy range (0.2-5 keV) novel seeding schemes (EEHG)

$$\varepsilon_{x,n}/\gamma \le \lambda/4\pi$$

$$\lambda = \lambda_U (1 + K^2/2)/(2\gamma^2)$$

Injector Baseline (0-100 MeV)



Beam requirements at the undulator

Electron energy	4.0	2.0-4.14	GeV
Bunch charge	100	10-300	рC
Repetition rate	0.62	0.93	MHz
Final norm. rms slice emittance	0.45	0.2-0.7	μm
Final peak current	1000	500-1500	Α
Final slice energy spread (rms)	500	125-1500	keV

Beam requirements at the injector exit (100 pC)

Peak current	12.0	А
Norm. rms emittance	0.35	μm
Higher-order <i>p</i> spread*	15.0	keV/c

^{*}the rms longitudinal momentum spread, taken after removing linear and quadratic correlations from the beam's longitudinal phase space

Multiobjective optimization: allows one to visualize tradeoffs between conflicting beam quality objectives

The Problem

Minimize $f_m(x_1, x_2, \ldots, x_n), \quad m = 1, \ldots M$

for
$$x_i^{(L)} \le x_i \le x_i^{(U)}, \quad i = 1, \dots, I$$

Subject to constraints of the form:

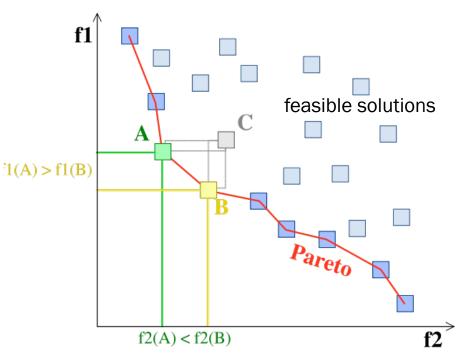
$$g_i(x_1, x_2, \dots, x_n) \ge 0, \quad j = 1, \dots, J$$

Example: Minimize transverse beam emittance and bunch length by tuning > 10 layout design settings.

A dominates B if A is not worse than B in all objectives, and is strictly better than B in at least one objective.

Pareto-optimal front: The set of all solutions that are not dominated by any other solution in the allowable search space.

Pareto Dominance



Example: A and B both dominate C, but A and B don't dominate each other.

Widely applied to injector*, linac, and ring design.

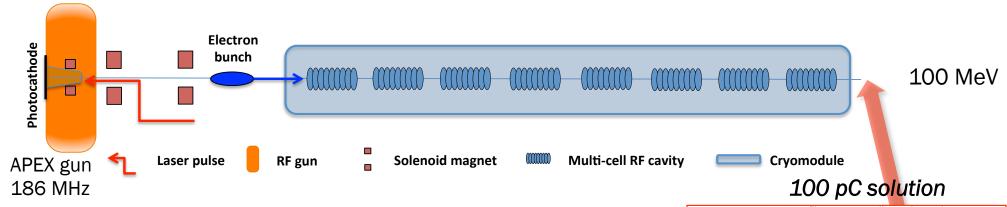
Comments on multiobjective optimization tools (1): algorithm details

Genetic Algorithm Approach (eg, NSGA-II or SPEA2)

- 1. Initialize population
- 2. Evaluate objective functions/constraints (beam dynamics simulation)
- 3. Assign fitness to all individuals, non-dominated solutions are preferred
- 4. Stochastically choose a subset for mating pool (higher fitness being preferred)
- 5. Apply crossing and mutation operators to generate offspring
 - Crossing: combine solutions to improve
 - Mutation: introduce randomness to investigate larger volume of parameter space
- 6. Evaluate objectives/constraints for the offspring
- 7. Repeat from step 3.
- ★ Population of non-dominated solutions 📥 approximation of the Pareto-optimal front.

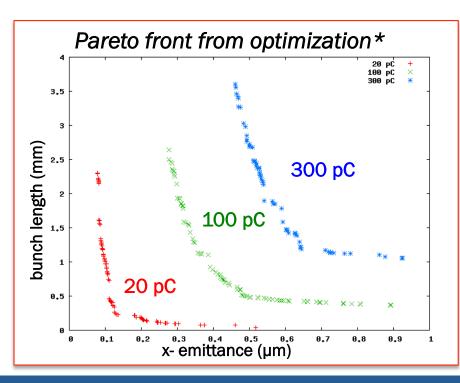


Comments on multiobjective optimization tools (2): an example from LCLS-II injector design



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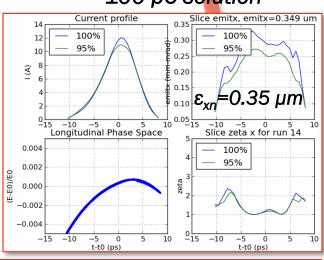
Science



8 knobs

2 objectives:

 ε_{xn} , σ_z



- Requires 100's of generations, ~ 1 week of computing time running in a cluster (80 cores).
- Allows us to compare optimized solutions for different layouts and different bunch charge.
- Requirements for the peak current and emittance are set by the downstream linac and FEL.

Applications to APEX and LCLS-II







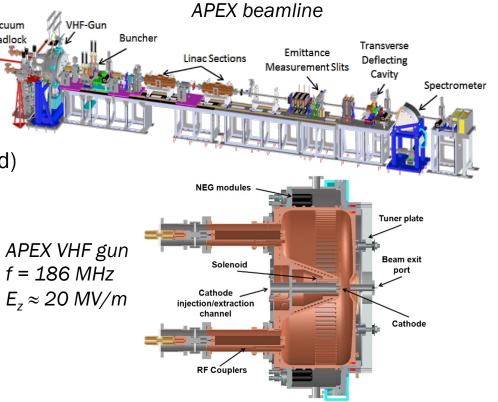
Multiobjective Genetic Optimization of APEX layout and design settings

Advanced Photoinjector Experiment (LBNL)

- The following 12 parameters are allowed to vary:
 - 1) the initial transverse rms beam size
 - 2) the initial pulse length FWHM
 - 3) the gun RF phase (the gun energy is held fixed)
 - 4-5) the buncher peak field and RF phase
 - 6-8) the three solenoid strengths
 - 9-10) the first cavity field and RF phase
 - 11-12) the second cavity field and RF phase
- There are two objectives:
 - 1) minimize transverse emittance at TCAV
 - 2) minimize bunch length at TCAV
- There are two constraints: rms energy spread < 200 keV, HOM $spread^* < 5$ keV/c
- For the beam profile at the cathode, we assume:

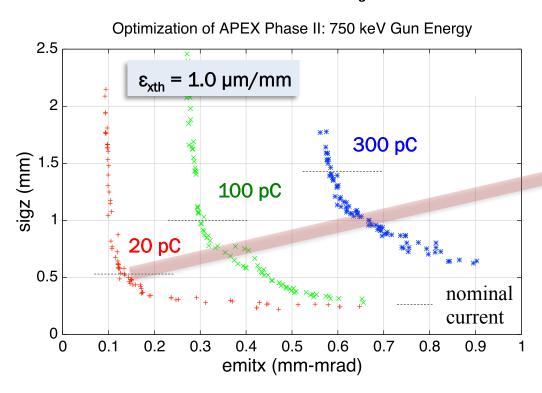
transversely - a Gaussian profile truncated at 1σ , longitudinally - a plateau w/2 ps rise time.

*the rms longitudinal momentum spread, taken after removing linear and quadratic correlations from the beam's longitudinal phase space



APEX Pareto-Optimal Performance (Nominal 750 keV Gun Energy)

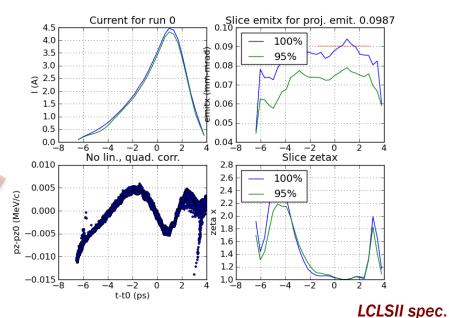
APEX Phase-II Injector



Simulation results are shown using 10K particles – this overestimates emittance in the 100 and 300 pC cases.

Demonstrated that the nominal APEX design could meet LCLS-II beam quality specifications.

20 pC solution (at the TCAV)



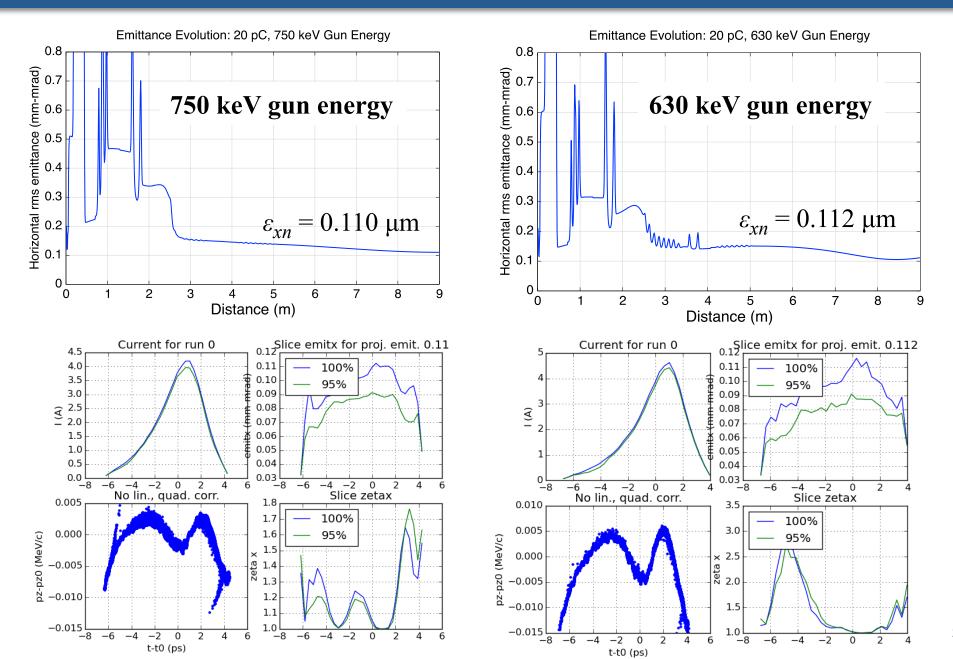
			<u>LCLSII spe</u>
Peak current	4.5	А	~5 A
Slice x-emittance	0.09	μm	
Proj. x-emittance	0.099	μm	<0.25 µm
Final energy	> 10	MeV	
Slice energy spread	< 1	keV	
Proj. energy spread	87	keV	
HOM spread	3.2	keV/c	<15 keV/c







Optimization Demonstrates that Comparable APEX 20 pC Performance can be Achieved at Lower Gun Energy



APEX 20 pC Optimization Near Experimental Settings: Optimization Settings and Procedure

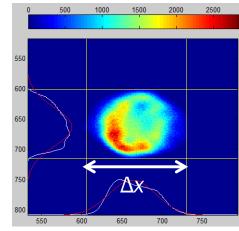
Due to practical considerations, APEX operation is simplified by running all cavities on-crest. Simulations indicate that this restriction can still produce solutions with $\sim 0.15 \ \mu m$ emittance.

To compare with measurement, we perform a new optimization in which the initial beam is *fixed* based on the measured rms properties of the laser at the cathode.

Initial distribution (20 pC):

Ideal gaussian truncated at $1\sigma_x$ with σ_x = 0.35 mm (before truncation) so σ_x = 156 μ m (after truncation). Thermal emittance: 0.6 μ m/mm. Plateau pulse with 14.3 ps FWHM.

Example 5 4 1



laser profile (100%)

 $\sigma_x = 156 \,\mu m$

 $\sigma_{\rm v}$ = 171 $\mu \rm m$

 $\Delta x = 0.80 \text{ mm}$

 $\Delta y = 0.74 \text{ mm}$

The following parameters are now allowed to vary during optimization:

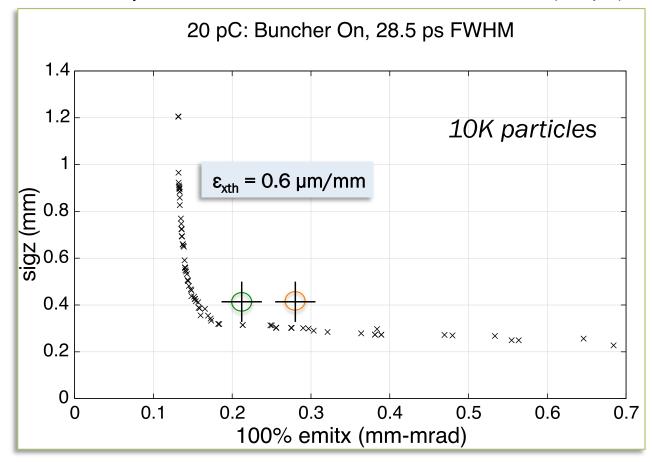
- 1) the gun RF phase (the gun energy is fixed at 630 keV)
- 2-3) the buncher peak field and RF phase
- 4-6) the three solenoid strengths
- 7-8) the first cavity field and RF phase
- 9-10) the second cavity field and RF phase





APEX 20 pC Optimization Near Experimental Settings: Comparison with Measurements

Pareto-Optimal Front Based on Simulation in Astra (20 pC)



In this optimization, the gun and cavities are forced to run on-crest.

Experimental data (20 pC):

100% Projected

$$\varepsilon_{xn} = 0.31 \pm 0.05 \ \mu m$$

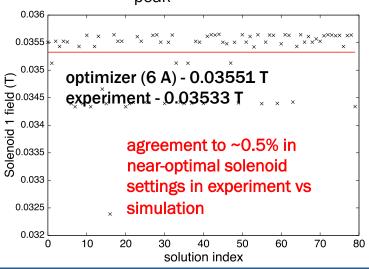
 $\varepsilon_{vn} = 0.25 \pm 0.06 \ \mu m$

95% Projected

$$\varepsilon_{xn} = 0.26 \pm 0.03 \, \mu m$$

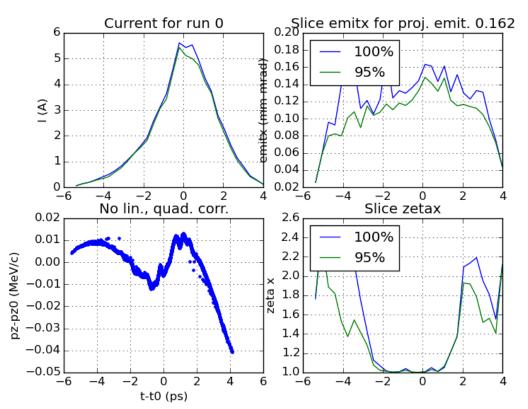
$$\varepsilon_{\rm vn}$$
 = 0.20 ± 0.04 µm

$$I_{\rm peak} \approx 6.5 \, {\rm A}$$

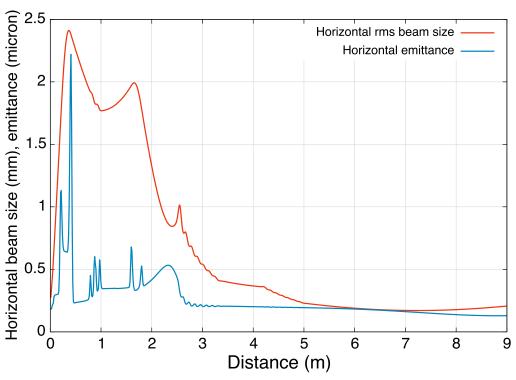


A Single APEX Solution at 20 pC Near Experimental Settings: Comparison with Measurements

Final Beam (at the TCAV)



Beam Size and Emittance



Peak current: 6 A (6.5 A)

Slice x-emittance: 0.15 µm

Proj. x-emittance: $0.162 \mu m (0.26 \mu m^*)$

Final energy: 15.7 MeV (15.7 MeV)

Slice energy spread: < 1 keV Proj. energy spread: 13.3 keV

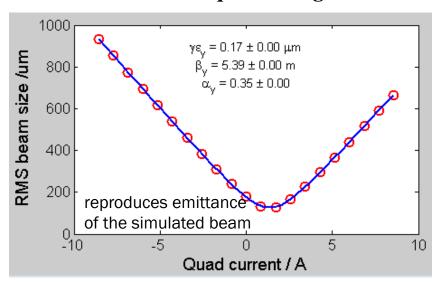
HOM spread: 7.7 keV/c



Quad Scan Emittance Measurements Affected by Space Charge in the Diagnostics Section

Simulated quad scan measurement

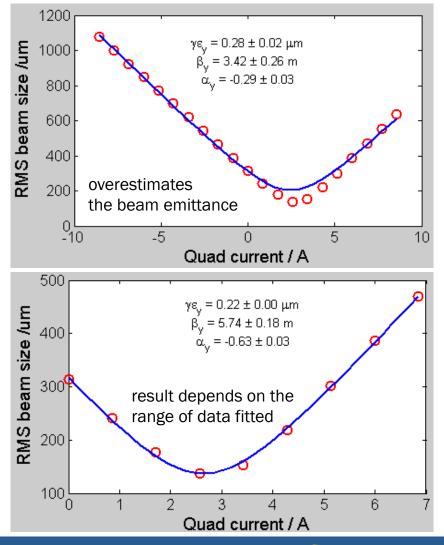
Without space charge



IMPACT-T was used to model the beam during the single-quad-scan emittance measurement, and the result was analyzed using the MATLAB tool.

The result ranges from 0.22-0.28 µm, depending on the range of data used for analysis.

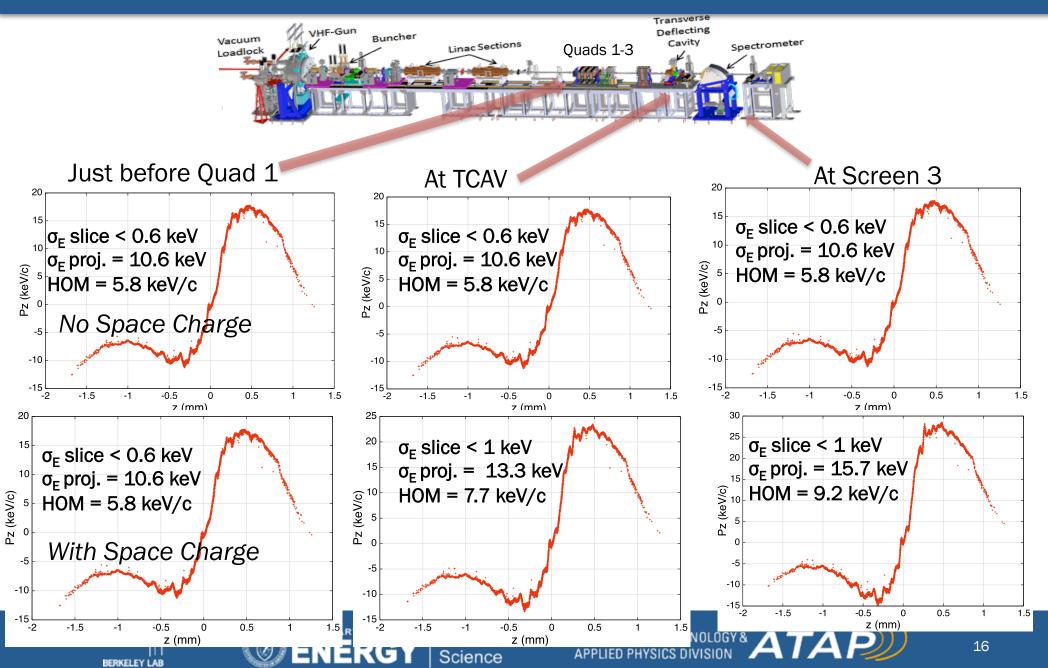
With space charge, 20 pC (6 A)



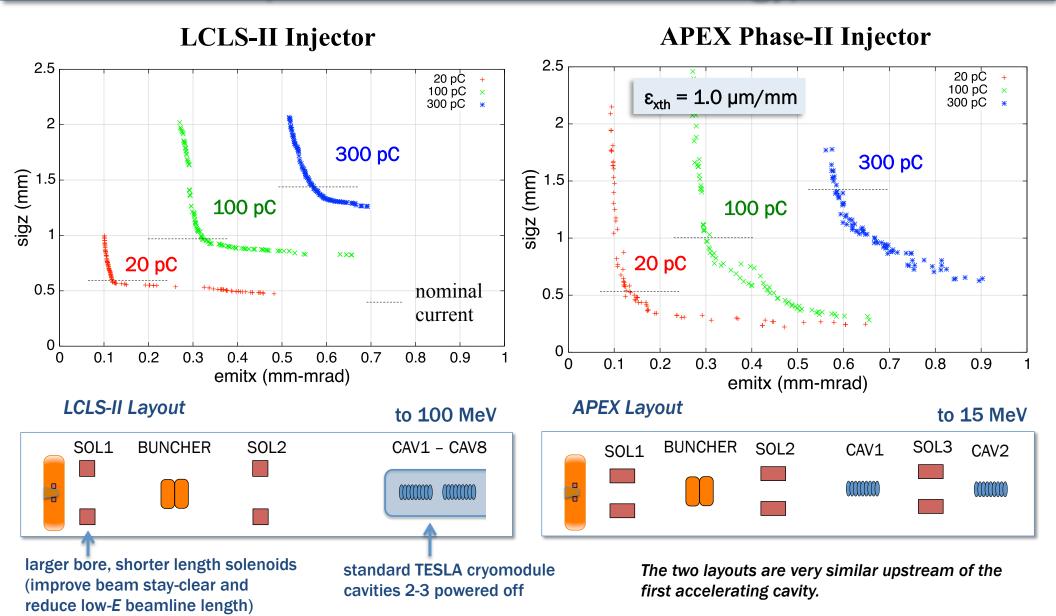




Space Charge Effects on Longitudinal Phase Space Evolution in the Diagnostics Section

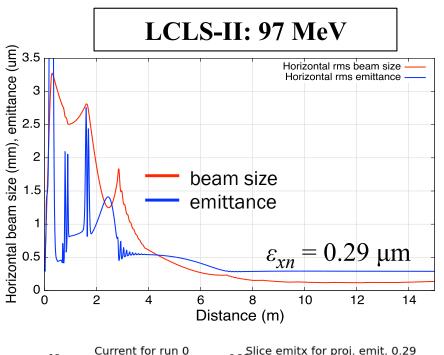


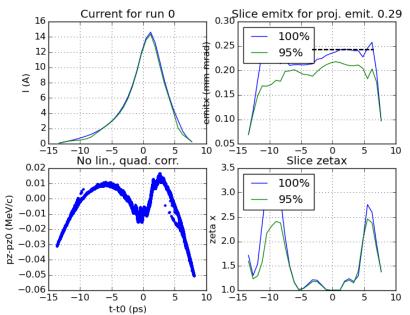
Comparison of APEX and LCLS-II Optimized Performance (Nominal 750 keV Gun Energy)

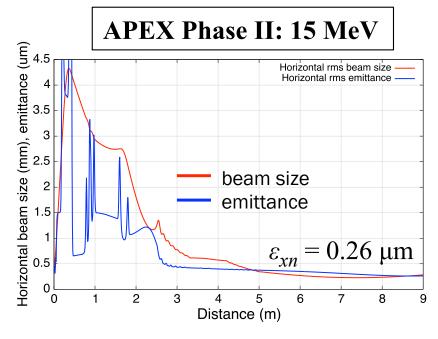


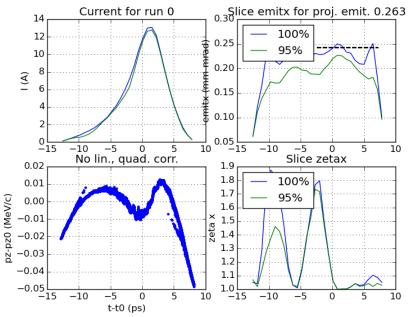
Simulation results are shown using 10K particles – this overestimates emittance in the 100 and 300 pC cases.

Comparison of LCLS-II and APEX 100 pC Optimized Solutions



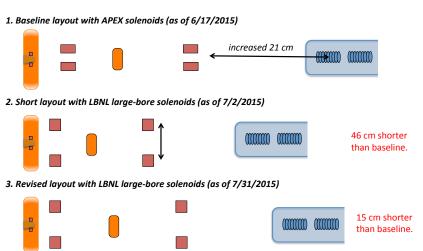


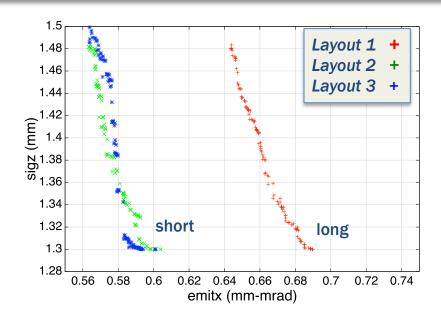




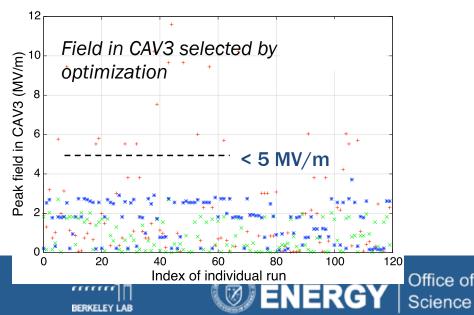
Using optimization to compare layout options and operation modes (examples for 300 pC)

Short drift length after SOL2 preferred

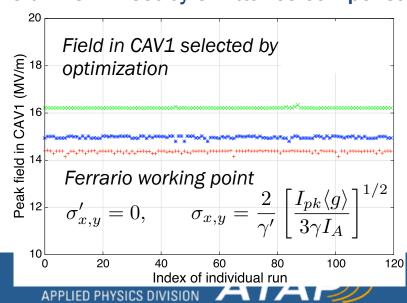




Operation with CAV2-3 powered off preferred



Field in CAV1 set by emittance compensation



An Example of Sensitivity to Constraints: Minimum Allowed Beam Energy at the Injector Exit

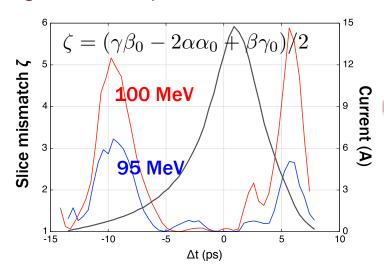
To avoid exceeding laser power constraints for the laser heater system, a lower bound is applied for the beam kinetic energy at the injector exit (exit of the first cryomodule): $W>W_{\min}$

This implies:
$$\sum_{j=1}^{N} \Delta W_j \geq W_{\min}, \quad \Delta W_j \leq \Delta W_{\max}$$

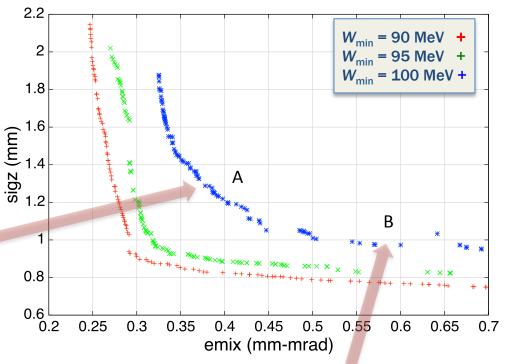
Cavity gradient and phase settings must satisfy:

$$qE_{\rm acc}L_{\rm acc}\cos\phi \ge W_{\rm min} - (N-1)\Delta W_{\rm max}$$

All cavities must be run with $E_{\rm acc} > 11.75$ MV/m, severely limiting emittance compensation.



Optimization of LCLS-II 100 pC performance for several values of energy constraint



All cavities must be run < 10° off-crest, severely limiting velocity compression.

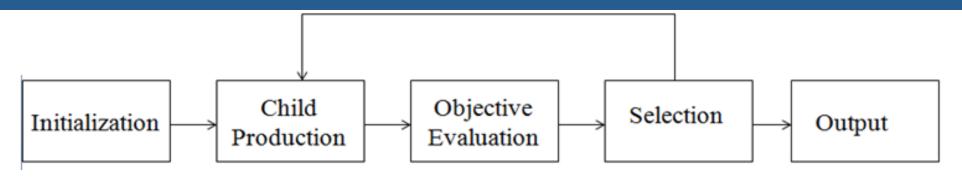
Additional developments







Differential Evolution: a rapidly-converging algorithm for global optimization



Differential Evolution Algorithm (single-objective optimization)

- A population of control parameter vectors is randomly generated from the control parameter space.
- A new perturbed vector \vec{v}_i is generated for each parent \vec{x}_i using one of several mutation strategies.
- A trial control parameter vector is generated by:

$$\vec{U}_i = (u_{i1}, u_{i2}, \dots, u_{iD})$$

$$u_{ij} = \begin{cases} v_{ij}, & \text{if } \operatorname{rand}_j \leq CR & \text{or } j = \operatorname{mbr}_i \\ x_{ij}, & \text{otherwise} \end{cases}$$

$$\operatorname{rand}_j \in [0, 1]$$

$$\operatorname{mbr}_i \in \{1, 2, \dots, D\}$$

• If the trial vector produces a better objective function value than \vec{x}_i , it will be put into the next generation. Otherwise, the original parent vector is kept in the next generation.

A Parallel Multi-Objective Differential Evolution Algorithm with Variable Population Size and External Storage (VPES-PMDE)

1. Define the minimum size, *NPmin* and the maximum size, *NPmax* of the parent population. Define the maximum size of external storage, *NPext*.

Ji Qiang

- 2. Generate an initial population of *NPini* parameter vectors randomly to uniformly cover the entire solution space.
- 3. Generate an offspring population using the differential evolutionary algorithm.



- 4. Check the new population against boundary conditions and constraints.
- 5. Combine the new population with the existing parent population from external storage and determine the non-dominated solutions (*Ndom*).
 - Move *min(Ndom, NPext)* solutions back into external storage. Pruning is used if *Ndom>NPext*.
 - Select NP parent solutions from this group of solutions for next generation production.
- 6. If $NPmin \le Ndom \le NPmax$, NP = Ndom. Otherwise, NP = NPmin if $Ndom \le NPmin$ and NP = NPmax if $Ndom \ge NPmax$.
- 7. If the stopping condition is met, stop. Otherwise, return to Step 3.



Unified Differential Evolution Shows Faster Convergence than NSGA-II for Benchmark Injector Test

Science

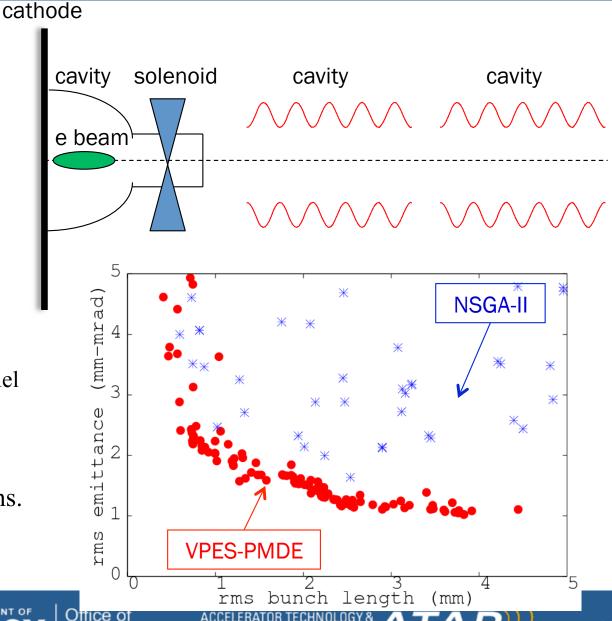
Control Parameters (10):

Initial laser transverse size and pulse length (2) Gun cavity phase (1) Solenoid strength and position (2) RF module starting position (1) Cavity 1 phase and amplitude (2) Cavity 2 phase and amplitude (2)

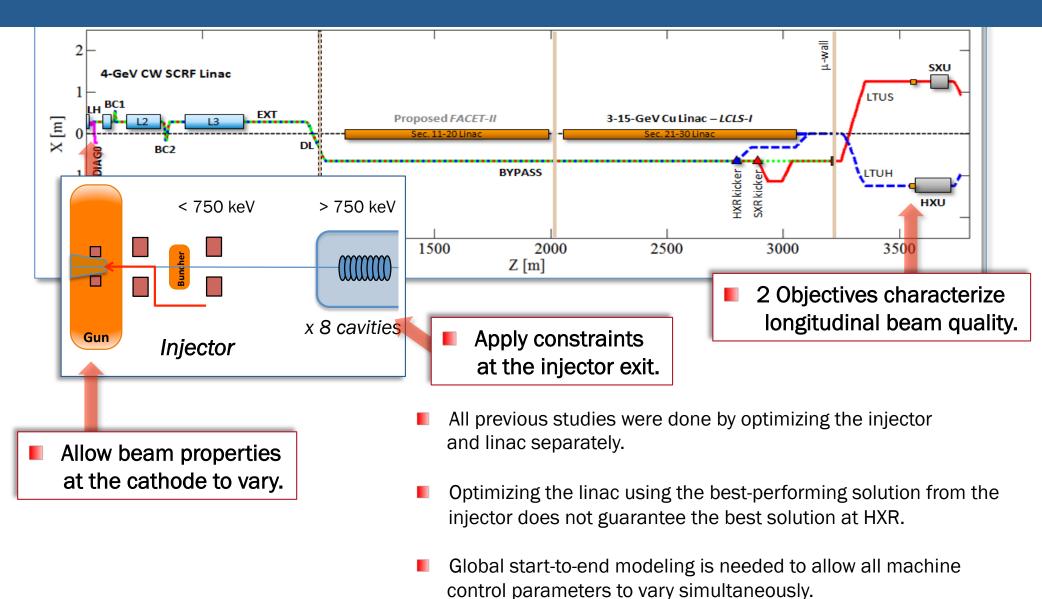
Two-level parallelization:

- each population member is a parallel execution of IMPACT-T (16 proc.)
- population size ~80

Comparison after 800 evaluations. (~ 30 min.)



Application: Multiobjective optimization of cathodeto-undulator performance for 20 pC charge in LCLS-II

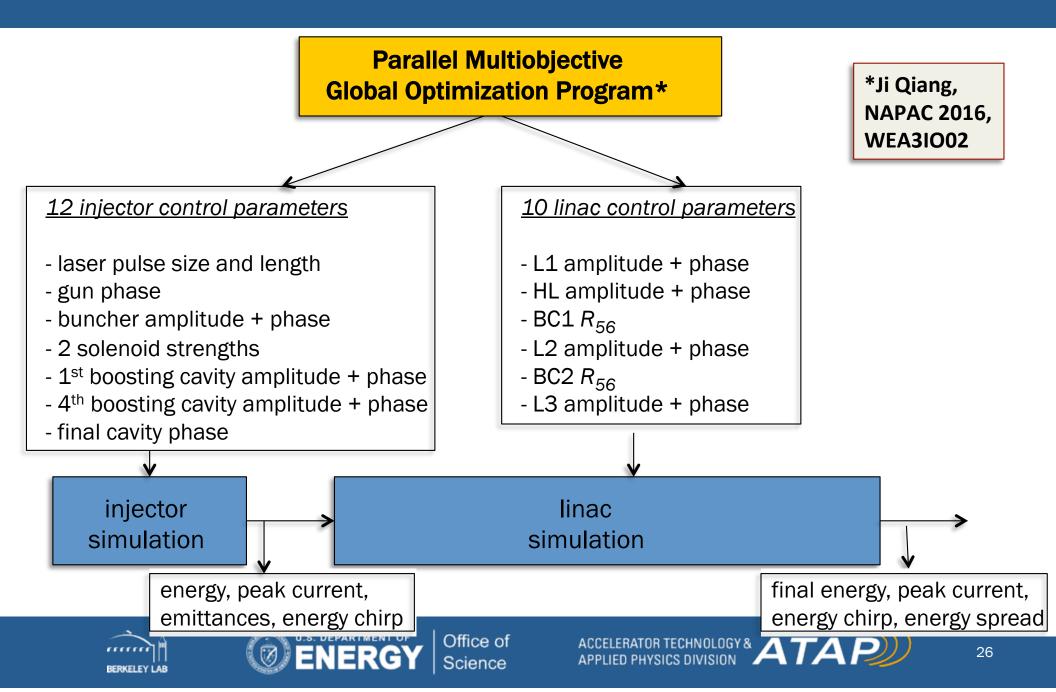




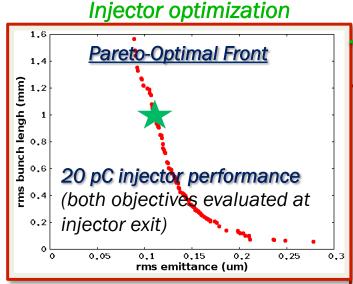




Application: Multiobjective optimization of cathodeto-undulator performance for 20 pC charge in LCLS-II

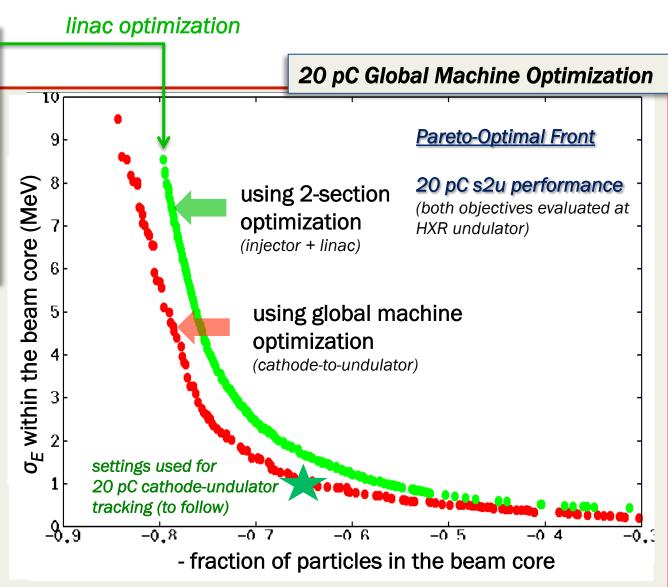


Application: Multiobjective optimization of cathodeto-undulator performance for 20 pC charge in LCLS-II



22 Control Parameters:

- 12 in the injector
- 10 in the linac
- A window is defined in the beam core [-7,9] μm.
- Global machine optimization gives better performance.



Conclusions

- Multiobjective optimization tools provide a robust method to search for globally optimum design settings the high-dimensional parameter space associated with high-brightness injector design that allows visualization of trade-offs between conflicting goals.
- An improved understanding of general design principles and the relevant beam physics can in some cases be "reverse-engineered" from the optimized solutions produced by such brute-force numerical tools.
- Care must be taken to apply these tools effectively: results can be sensitive to choice of optimization parameters, constraints, and allowed parameter ranges.
- These tools played a critical role in injector beam dynamics studies for both APEX and LCLS-II, and rapid advances in the efficiency of optimization algorithms* will make high-fidelity optimization based on beam dynamics simulation increasingly accessible.
- Global optimization using start-to-undulator simulation can provide significant gains in FEL performance over two-stage optimization of injector and linac separately.

Acknowledgments

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