Optimization via adjoint methods of flat-to-round transformers for electron cooling

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Adjoint Approach: What it does

- Finds the dependence of system performance on parameters
- Useful for:

Optimization – gradient descent Sensitivity Studies

- Requires identification of a Figure of Merit (FoM)
 - $F(\mathbf{a})$ where **a** Vector of parameters

- Efficient calculation of $dF(\mathbf{a})/d\mathbf{a}$

Direct evaluation w/N parameters, requires N solutions Adjoint approach – One or two solutions

How Does It Work?

X - State of System **a** - Vector of Parameters

A(X) = a Nonlinear vector Figure of Merit (FoM) equation F(X,a)

Linearize: $\mathbf{a} \to \mathbf{a} + \delta \mathbf{a}$ $\mathbf{X} \to \mathbf{X} + \delta \mathbf{X}$ $F \to F + \delta F$ $\delta F = \delta \mathbf{a} \cdot \frac{\partial F}{\partial \mathbf{a}} + \delta \mathbf{X} \cdot \frac{\partial F}{\partial \mathbf{X}}$ $\delta \mathbf{X} \cdot \frac{\partial \mathbf{A}}{\partial \mathbf{X}} (\mathbf{X}) = \delta \mathbf{a}$ Solve Adjoint $\frac{\partial \mathbf{A}}{\partial \mathbf{X}} \cdot \mathbf{Y} = \frac{\partial F}{\partial \mathbf{X}}$ $\delta F = \delta \mathbf{a} \cdot \left[\frac{\partial F}{\partial \mathbf{a}} + \mathbf{Y}\right]$

Optimization of Flat to Round Transformers Using Adjoint Techniques*

L. Dovlatyan, B. Beaudoin, S. Bernal, I. Haber, D. Sutter and T. M. Antonsen Jr, Phys Rev Accel and Beams V25, 044002 (2022).



Flat to Round and Round to Flat transformers were proposed for cooling of hadron beams. Ya. Derbenev, Adapting optics for high-energy electron cooling, Tech. Rep. UM-HE-98-04-A (1998).

Steps

1. Derive system of moment equations (include self fields)

2. Linearize (to compute parameter gradient)

- 3. Find adjoint system
- 4. Decide on Figures of Merit
- 5. Optimize by Gradient Descent



Moment Equations

The second order moments are averages of the 4 by 4 elements of the Sigma matrix.

10 independent moments

$$\underline{\Sigma} = \begin{bmatrix} \begin{pmatrix} xx & xx' & xy & xy' \\ x'x & x'x' & x'y & x'y' \\ yx & yx' & yy & yy' \\ y'x & y'x' & y'y & y'y' \end{pmatrix} \\ x' = \frac{dx}{dz}$$



Moment-PIC Comparison for FTR



Linearization to Calculate Gradient in Parameter Space - a Base case: $\frac{d}{dz}\mathbf{X} = \mathbf{O}_{magnets}(z|\mathbf{a}) \cdot \mathbf{X}(z) + \mathbf{O}_{SpCh}(\mathbf{X}) \cdot \mathbf{X}(z)$ $\mathbf{A} \rightarrow \mathbf{a} + \delta \mathbf{a}$ Direct variation: $\frac{d}{dz}\delta\mathbf{X}^{(X)} = \left[\mathbf{O}_{magnets} + \mathbf{O}_{SpCh}\right] \cdot \delta\mathbf{X}^{(X)} + \left(\delta\mathbf{a} \cdot \frac{\partial}{\partial \mathbf{a}}\mathbf{O}_{magnets} + \delta\mathbf{X}^{(X)} \cdot \frac{\partial}{\partial \mathbf{X}}\mathbf{O}_{SpCh}(\mathbf{X})\right) \cdot \mathbf{X}(z)$ $0 = \left. \delta \mathbf{X}^{(X)} \right|_{z}$ Change in FoM: $\delta F = \delta \mathbf{X}^{(X)} \Big|_{z} \cdot \frac{\partial F}{\partial \mathbf{Y}}$ $\frac{d}{d\tau} \delta \mathbf{X}^{(Y)} = \left[\mathbf{O}_{magnets} + \mathbf{O}_{SpCh} \right] \cdot \delta \mathbf{X}^{(Y)} + \delta \dot{\mathbf{X}}^{(Y)}$ Adjoint equation: TRD $\left. \delta \mathbf{X}^{(Y)} \right|_{z} \leftarrow \text{TBD}$ Final condition:

Adjoint Magic – Can Show...

Adjoint equation:
$$\frac{d}{dz} \delta \mathbf{X}^{(Y)} = \begin{bmatrix} \mathbf{O}_{magnets} + \mathbf{O}_{SpCh} \end{bmatrix} \cdot \delta \mathbf{X}^{(Y)} + \delta \dot{\mathbf{X}}^{(Y)}$$
Integrated backward in z
F - Figure of Merit
Final condition:
$$\delta \mathbf{X}^{(Y)} \Big|_{z_{f}} \cdot \hat{\mathbf{J}} = \frac{\partial F}{\partial \mathbf{X}} \qquad \hat{\mathbf{J}} = \text{Matrix of zeros and ones}$$

$$\delta F = \int_{z_{f}}^{z_{f}} dz \, \delta \mathbf{X}^{(Y)} \cdot \delta \mathbf{a} \cdot \frac{\partial}{\partial \mathbf{a}} \mathbf{O}_{magnets} \cdot \mathbf{X}(z)$$
Base case
Change in FOM
Change in Magnet Parameters
Sensitivity function

Figure of Merit and Gradient

$$FoM = \frac{1}{2} \sum_{Terms-i} T_{i}$$

 T_1 - beam is round T_2 - radius is locally constant T_3 - velocity space is isotropic T_4 - radial force balance T_5 - rigid rotation

11 Parameters

Location of 4 magnets Strength of 4 magnets Orientation of 3 Quads



Optimization Results

10

8

6

4

2

0

 x_{rms}^2

 y_{rms}^2

0.05

0.00

μm²



Continuous magnetic field profiles



0.15

0.10

5mA

1mA

0mA

0.20

fixed rotation (45°) varied rotation

0.30

0.25

0mA

1mA

5mA

Alternate FoMs



FoM includes radial force balance

FoM includes transverse energy density in lab frame

Integrated FoMs also possible

$$F = \int dz f(\mathbf{X}, z)$$

Demonstration of Flat/Round Transformations of Angular Momentum and Space Charge Dominated Electron Beams



Slit



Generation of highly asymmetric beams

SLIT: L × H	BEAM CURRENT	$ ilde{m{arepsilon}}_x, ilde{m{arepsilon}}_y$	$\tilde{arepsilon}_x ig/ ilde{arepsilon}_y$
10 × 0.2 mm	0.60 mA	53 μm, 1.1 μm	50
10 × 0.5 mm	1.4 mA	53 μm, 2.7 μm	20
10 × 1.0 mm	2.9 mA	53 μm, 5.3 μm	10

Adjoint Relations for Particle Description

TMA, D. Chernin, J. Petillo, Phys. Plasmas 26, 013109 (2019)

Base Solution + Perturbation

$$(\mathbf{x}_{j},\mathbf{p}_{j}) \rightarrow (\mathbf{x}_{j},\mathbf{p}_{j}) + (\delta \mathbf{x}_{j},\delta \mathbf{p}_{j})$$

$$\rho(\mathbf{x}) \to \rho(\mathbf{x}) + \delta \rho(\mathbf{x})$$
$$\Phi_T(\mathbf{x}) \to \Phi_T(\mathbf{x}) + \delta \Phi_T(\mathbf{x})$$

 $\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}$ $\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}$

<u>Two Linearized Solutions</u> $[\delta x_{j}(t), \delta p_{j}(t)]$ true $[\delta \hat{x}_{j}(t), \delta \hat{p}_{j}(t)]$ adjoint

$$\delta \Phi_T = \delta \Phi - \frac{v_z}{c} \delta A_z \leftrightarrow$$
 Includes focusing magnets

Change in symplectic area

Perturbed fields on boundary

$$\sum_{j} I_{j} \left(\delta \hat{\mathbf{p}}_{j} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \delta \hat{\mathbf{x}}_{j} \right) \Big|_{0}^{L} = -q \varepsilon_{0} \int_{S} da \mathbf{n} \cdot \left[\delta \Phi_{T} \nabla \delta \hat{\Phi}_{T} - \delta \hat{\Phi}_{T} \nabla \delta \Phi_{T} \right]$$

Adjoint Treatment of Particle Equations

Change in symplectic area

Perturbed fields on boundary

$$\sum_{j} I_{j} \left(\delta \hat{\mathbf{p}}_{j} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \delta \hat{\mathbf{x}}_{j} \right) \Big|_{0}^{L} = -q \varepsilon_{0} \int_{S} da \mathbf{n} \cdot \left[\delta \Phi_{T} \nabla \delta \hat{\Phi}_{T} - \delta \hat{\Phi}_{T} \nabla \delta \Phi_{T} \right]$$

Pick:
$$\left(\delta \hat{\mathbf{p}}_{j}, \delta \hat{\mathbf{x}}_{j} \right)_{z=L} \right)$$

Integrate backward in z

$$\delta F = \sum_{j} \left(\frac{\partial F}{\partial \mathbf{x}_{j}} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \left(-\frac{\partial F}{\partial \mathbf{p}_{j}} \right) \right) \Big|_{L} = -q \varepsilon_{0} \int_{S} da \mathbf{n} \cdot \left[\delta \Phi_{T} \nabla \delta \hat{\Phi}_{T} \right]$$

Change in FoM
Arb. $F(\mathbf{x}, \mathbf{p}, \mathbf{z}_{f})$
Change in focusing magnets. Includes multipole variation
Change in focusing magnets. Sensitivity

Circular Accelerators-Periodicity?



Optimize FoM subject to periodicity

Constrained Optimization "Adjoint with a Chaser"

Summary slide, 5th ICFA mini-workshop on Space Charge Theme: Bridging the gap in space charge dynamics

Adjoint methods are a powerful way to evaluate parameter dependences in many systems involving charged particle dynamics.

Application to 2nd-moments has been implemented. Need to develop applications to particle distributions. Optimize phase space distributions, circular Accelerators.

Adjoint relation is a consequence of retaining self-fields.

Theory Perspective: Space Charge – Good.

Moment Equations

Transverse phase space:

$$x, x' = \frac{dx}{dz}, y, y' = \frac{dy}{dz}$$

The second order moments are averages of the 4 by 4 elements of the Sigma matrix.

$$\underline{\Sigma} = \begin{bmatrix} xx & xx' & xy & xy' \\ x'x & x'x' & x'y & x'y' \\ yx & yx' & yy & yy' \\ y'x & y'x' & y'y & y'y' \end{bmatrix}$$

Moments: $\mathbf{Q}, \mathbf{P}, \mathbf{E}, L$

$$\mathbf{Q} = \begin{pmatrix} Q_{+} \\ Q_{-} \\ Q_{x} \end{pmatrix} = \begin{pmatrix} \langle x^{2} + y^{2} \rangle / 2 \\ \langle x^{2} - y^{2} \rangle / 2 \\ \langle xy \rangle \end{pmatrix} \mathbf{P} = \frac{d}{dz} \mathbf{Q} = \begin{pmatrix} P_{+} \\ P_{-} \\ P_{x} \end{pmatrix} = \begin{pmatrix} \langle xx' + yy' \rangle \\ \langle xx' - yy' \rangle \\ \langle yx' + xy' \rangle \end{pmatrix}_{\mathbf{E}} = \begin{pmatrix} E_{+} \\ E_{-} \\ E_{x} \end{pmatrix} = \begin{pmatrix} \langle x'^{2} + y'^{2} \rangle \\ \langle x'^{2} - y'^{2} \rangle \\ 2 \langle y'x' \rangle \end{pmatrix}$$

Angular momentum $L = \langle xy' - yx' \rangle$

Linearized System

Linear perturbation due to true change in parameters

Adjoint system

Base case

$$\frac{d}{dz} \delta \mathbf{Q}^{(Y)} = \delta \mathbf{P}^{(Y)}$$
$$\frac{d}{dz} \delta \mathbf{P}^{(Y)} = \delta \mathbf{E}^{(Y)} + \mathbf{O} \cdot \delta \mathbf{Q}^{(Y)}$$
$$\frac{d}{dz} \delta \mathbf{E}^{(Y)} = \mathbf{O} \cdot \delta \mathbf{P}^{(Y)} + \mathbf{N} \delta L^{(Y)} + \delta \dot{\mathbf{E}}^{(Y)}$$
$$\frac{d}{dz} \delta L^{(Y)} = -\mathbf{N}^{\dagger} \cdot \delta \mathbf{Q}^{(Y)}$$

$$\delta FoM = \int_{z_i}^{z_f} dz \Big\{ \delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{Q} + \delta L^{(Y)} \mathbf{Q} \cdot \delta \mathbf{N}_{Q,B}^{(X)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{P} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{N}_{Q,B}^{(X)} L \Big\}$$

Change in magnet parameters

Figure of Merit and Gradient

0.4

0.2

0.0

-0.2

-0.4

-0.6

-0.8

0.05

0.00

A FOM

 K_{q1}

K_{q3}

-0.04

-0.02

0.00

 $\Delta K_q \; (1/m^2)$

 K_{q2}

Adjoint calculation

0.02

Direct measurement

0.04

Constant radius, Round

$$F = \frac{1}{2} \left[\left| \mathbf{P} \right|^2 + k_0^2 \left(Q_-^2 + Q_x^2 \right) + k_0^{-2} \left(E_-^2 + E_x^2 \right) \right]$$

$$+\frac{1}{2}\left[k_{0}^{-2}\left(E_{+}-\frac{1}{2}k_{\Omega}^{2}Q_{+}+\Lambda\right)^{2}+\left(2E_{+}Q_{+}-L^{2}\right)^{2}\right]$$

Radial force balance, Rigid rotation

$$\mathbf{Q} = \begin{pmatrix} \frac{1}{2} \langle x^2 + y^2 \rangle \\ \frac{1}{2} \langle x^2 - y^2 \rangle \\ \langle xy \rangle \end{pmatrix} \mathbf{P} = \begin{pmatrix} \langle xx' + yy' \rangle \\ \langle xx' - yy' \rangle \\ \langle yx' + xy' \rangle \end{pmatrix} \mathbf{E} = \begin{pmatrix} \langle x'^2 + y'^2 \rangle \\ \langle x'^2 - y'^2 \rangle \\ 2 \langle y'x' \rangle \end{pmatrix}^{-0.15} \xrightarrow{-0.03 \quad -0.02 \quad -0.01 \quad 0.00 \quad 0.01 \quad 0.02 \quad 0.03}{\Delta k_{\Omega}^2 (\mathbf{G}/\mathbf{rad})}$$

Optimization – Space Charge Compensation



Global Beam Sensitivity Function for Electron Guns

Goal

Derive and Calculate a function that gives the variation of <u>specific beam parameters</u> to

- variations in <u>electrode potential/position</u>
- variations in magnet current/position

Can be used to

- establish manufacturing tolerances
- optimize gun designs

Should be embedded in gun code (e.g. Michelle)

Thermionic Cathode Electron Gun



What shape to make electrodes?



Michelle: Petillo, J; Eppley, K; Panagos, D; et al., IEEE TPS 30, 1238-1264 (2002).

Code (Michelle) solves the following equations:

Equations of motion for N particles j=1,N

Start with vacuum fields

$$\frac{dx_{j}}{dt} = \frac{\partial H}{\partial p} \qquad \frac{dp_{j}}{dt} = -\frac{\partial H}{\partial x}$$
Accumulates a charge density
$$\rho(x) = \sum_{j} I_{j} \int_{0}^{T_{j}} dt \, \delta(x - x_{j}(t))$$
Solves Poisson Equation
$$-\nabla^{2} \Phi = \rho / \varepsilon_{0}$$

Sensitivity Function



Direct Approach:

Do many simulations with different anode potentials, positions

Select the best based on some metric measured at the exit.





Reference Solution + Two Linearized Solutions

$$\begin{pmatrix} \mathbf{x}_{j}, \mathbf{p}_{j} \end{pmatrix} \rightarrow \begin{pmatrix} \mathbf{x}_{j}, \mathbf{p}_{j} \end{pmatrix} + \begin{pmatrix} \delta \mathbf{x}_{j}, \delta \mathbf{p}_{j} \end{pmatrix}$$

$$\rho(\mathbf{x}) \rightarrow \rho(\mathbf{x}) + \delta \rho(\mathbf{x})$$

$$\Phi(\mathbf{x}) \rightarrow \Phi(\mathbf{x}) + \delta \Phi(\mathbf{x})$$

Two Linearized Solutions

 $[\delta x_{i}(t), \delta p_{i}(t)]$ true

 $[\delta \hat{x}_{j}(t), \delta \hat{p}_{j}(t)]$ adjoint

Reference Solution

Perturbation

subject to different BC's

Can show

$$\sum_{j} I_{j} \left(\delta \hat{\mathbf{p}}_{j} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \delta \hat{\mathbf{x}}_{j} \right) \Big|_{0}^{T_{j}} = -q \varepsilon_{0} \int_{S} da \mathbf{n} \cdot \left[\delta \Phi \nabla \delta \hat{\Phi} - \delta \hat{\Phi} \nabla \delta \Phi \right]$$

Generalized Green Theorem

Generalized Green's Theorem

$$\sum_{j} I_{j} \left(\delta \hat{\mathbf{p}}_{j} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \delta \hat{\mathbf{x}}_{j} \right) \Big|_{0}^{T_{j}} = -q \varepsilon_{0} \int_{S} da \mathbf{n} \cdot \left[\delta \Phi \nabla \delta \hat{\Phi} - \delta \hat{\Phi} \nabla \delta \Phi \right]$$

Problem #1 (true problem) Unperturbed trajectories at cathode, Perturbed potential on boundary. $\delta n = 0, \quad \delta x = 0, \quad \delta \Phi(\mathbf{x}) \neq 0$

$$\left. \frac{\delta \hat{p}_{j}}{T} \right|_{T} = \lambda \mathbf{x}_{\perp j}, \quad \left. \frac{\delta x_{j}}{T} \right|_{T} = 0, \quad \delta \hat{\Phi}(\mathbf{x}) = 0$$

$$\lambda IR_{RMS} \delta R_{RMS} = \lambda \sum_{j} I_{j} \left(\mathbf{x}_{j} \cdot \delta \mathbf{x}_{j} \right) \Big|_{T_{j}} = -q \varepsilon_{0} \int_{S} da \,\delta \Phi \left(\mathbf{n} \cdot \nabla \delta \hat{\Phi} \right)$$

Sensitivity Function

Vertical Displacement of the Beam



Predicted displacement / Calculated displacement = 0.9969



Recent Adjoint Approaches

- <u>Beam optics sensitivity function</u>, TMA, D. Chernin, J. Petillo, Phys. Plasmas 26, 013109 (2019); doi: 10.1063/1.5079629
- <u>Stellarator Optimization and Sensitivity</u>, E. Paul, M. Landreman, TMA, *J. Plasma Phys*. (2019), vol. 85, 905850207, *J. Plasma Phys*. (2021), vol. 87, 905870214
- <u>Optimization of Flat to Round Transformers in Particle</u> <u>Accelerators</u>, L. Dovlatyan, B. Beaudoin, S. Bernal, I. Haber, D. Sutter and TMA, Phys Rev Accel and Beams V25, 044002 (2022).
- <u>Adjoint Equations for Beam-Wave Interaction and</u>
 <u>Optimization of TWT Design</u>, A. Vlasov, TMA, D. Chernin and I.
 Chernyavskiy, IEEE Trans. Plasma Sci. V. March (2022).

Give a child a hammer and everything becomes a nail.

Basic Adjoint Example Jackson, Classical Electrodynamics Problems 1.12 and 1.13

A charge q is placed at an arbitrary point, \mathbf{x}_0 , relative to two grounded, conducting electrodes.



What is the charge q_1 on the surface of electrode 1?

Repeat for different x₀

Solution – Green's Reciprocation Theorem

$$\frac{\operatorname{Prob} \#1}{\operatorname{Direct}} \quad \nabla^2 \phi = -q \delta(\mathbf{x} - \mathbf{x}_0) \quad \text{BC:} \quad \phi \big|_{B_1} = \phi \big|_{B_2} = \phi(x \to \infty) = 0$$
evaluation
$$q_1 = \int_{B_1} d^2 x \, \mathbf{n} \cdot \nabla \phi \quad \text{Repeated for each } \mathbf{x}_0$$

Prob #2
Adjoint Problem
$$\nabla^2 \psi = 0$$
BC: $\psi |_{B1} = 1, \quad \psi |_{B2} = \psi(x \to \infty) = 0$
Done onceGreen's
Theorem $\int_{V} d^3 x (\psi \nabla^2 \phi - \phi \nabla^2 \psi) = \int_{S} d^2 x n \cdot (\psi \nabla \phi - \phi \nabla \psi)$
 0 $\int_{V} 0$ When the dust settles: $-q \psi(\mathbf{x}_0) = q_1$