### Adjoint Methods in Charged Particle Dynamics

or

When the solution to your problem is not your problem.

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### 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 x<sub>0</sub>

#### Solution – Green's Reciprocation Theorem

Prob #1 
$$\nabla^2 \phi = -q \delta(\mathbf{x} - \mathbf{x}_0)$$
 BC:  $\phi|_{B1} = \phi|_{B2} = \phi(x \to \infty) = 0$   
Your  
Problem  $q_1 = \int_{B1} d^2 x \, \mathbf{n} \cdot \nabla \phi$ 

Prob #2  
Adjoint (Not
$$\nabla^2 \psi = 0$$
BC: $\psi |_{B1} = 1, \quad \psi |_{B2} = \psi (x \rightarrow \infty) = 0$ your) Problem

Green' s Theorem

$$d^{3}x(\psi\nabla^{2}\phi - \phi\nabla^{2}\psi) = \int d^{2}x n \cdot (\psi\nabla\phi - \phi\nabla\psi)$$
  
os:  
$$-q\psi(\mathbf{x}_{0}) = q_{1}$$

When the dust settles:

### George Green 1793-1841

# **The Green of Green Functions**

In 1828, an English miller from Nottingham published a mathematical essay that generated little response. George Green's analysis, however, has since found applications in areas ranging from classical electrostatics to modern quantum field theory.

his family built a house next to the mill, Green spent most of his days and many of his nights working and indeed living in the mill. When he was 31, Jane Smith bore him a daughter. They had seven children in all but never married. It was said that Green's father felt that Jane was not a suitable

Lawrie Challis and Fred Sheard Physics Today Dec. 2003man and landowner and threatened to

disinherit him.

- Born in Nottingham (Home of Robin Hood)
- Father was a baker
- At age 8 enrolled in Robert Goodacre's Academy
- Left after 18 months (extent of formal education pre age 40)
- Worked in bakery for 5 years
- Sent by father to town mill to learn to be a miller

- Fell in love with Jane, the miller's daughter.
- Green's father forbade marriage.
- Had 7 children with Jane.
- Self published work in 1828
- With help, entered Cambridge 1833, graduated 1837.
- Theory of Elasticity, refraction, evanescence
- "Discovered" by Lord Kelvin in 1840.
- Died of influenza, 1841



Green's Mill: still functions

# Features of Problems Suited to an Adjoint Approach

- Many computations need to be repeated. (many different locations of charge, q)
- 2. Only a limited amount of information about the solution is required.(only want to know charge on electrode #1)

# Relation to Reciprocity

#### **Example:**

- Antenna sending and receiving radiation patterns are equal due to time reversal symmetry of ME.

- Direct calculation of receiving pattern requires many simulations
- Instead, calculate sending pattern and invoke reciprocity



### Other Examples of Reciprocity

Electrostatics Symmetry of the Capacitance Matrix

Electromagnetics Symmetry of the Inductance Matrix Symmetry of Scattering Matrix

Collisional Transport: Onsager Symmetry of off-diagonal elements of transport matrices.

Temperature gradient	→	Electric current	
Electric field	→	Heat flux	
Neoclassical Tokamak Transport			
Pressure gradient	→	Bootstrap Current	
Toroidal E-field	→	Ware particle flux	

### Adjoint Methods in Engineering

Journal of The Electrochemical Society, 164 (11) E3232-E3242 (2017)



E3232

JES FOCUS ISSUE ON MATHEMATICAL MODELING OF ELECTROCHEMICAL SYSTEMS AT MULTIPLE SCALES IN HONOR OF JOHN NEWMAN

#### Adjoint Method for the Optimization of the Catalyst Distribution in Proton Exchange Membrane Fuel Cells

James Lamb,<sup>a,b</sup> Grayson Mixon,<sup>a,b</sup> and Petru Andrei<sup>a,b,\*,z</sup>

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# Adjoint method for the optimization of insulated gate bipolar transistors

Cite as: AIP Advances 9, 095301 (2019); doi: 10.1063/1.5113764 Submitted: 7 June 2019 • Accepted: 23 August 2019 • Published Online: 3 September 2019



# Adjoint shape optimization applied to electromagnetic design

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#### Courtesy, Elizabeth Paul

#### Adjoint methods for car aerodynamics

Carsten Othmer 🖾

Journal of Mathematics in Industry 2014 4:6 DOI: 10.1186/2190-5983-4-6 © Othmer; licensee Springer. 2014 Received: 30 March 2013 Accepted: 5 March 2014 Published: 3 June 2014



Super Computer

#### 1985 Volvo 240 DL



Oops, coding error.

### Adjoint Approach in Plasma and Beam Physics

- <u>Neoclassical Transport</u>, F. Hinton, and R. Hazeltine, Rev. Mod Phys, 48 (2), 1976
- <u>Calculation of beam driven currents in magnetized plasmas</u>, S. Hirshman, PoF, 23, 1238 (1980).
- <u>Calculation of RF current drive in magnetic confinement</u> <u>plasma configurations</u>, TMA and K. Chu PoF 25, (1982)
- <u>Calculation of RF induced transport in magnetic confinement</u> <u>plasmas</u>, TMA and K. Yoshioka, PoF 29, (1986), Nucl. Fusion, 26 (1986).
- <u>Shot noise on gyrotron beams</u>, TMA, W. Manheimer and A. Fliflet, PoP (2001).

### **RF** Current Drive in Fusion Plasmas

#### Magnetic Confinement: ITER

US-EU-Russia-Japan-India Collaboration Will be built in Cardarache France Completion 2016?? http://www.iter.org/





Injecting RF waves can drive a toroidal current. N. Fisch PRL (1978)

# **RF** Current Drive Efficiency

Original Langevin Treatment: Nat Fisch, PRL (1978)

RF pushes particles in velocity space.

Collisions relax distribution back to equilibrium.

What is the current generated per unit power dissipated? J/P<sub>D</sub>

$$J = \int d^3 v \,\vec{\Gamma} \cdot \frac{\partial}{\partial v} \Psi \qquad P_D = \int d^3 v \,\vec{\Gamma} \cdot \frac{\partial}{\partial v} \mathcal{E}$$

 $\psi$  inversely proportional to collision rate

 $\vec{\Gamma}$  = RF induced velocity space particle flux

### **RF** Current Drive Efficiency

RF pushes particles in velocity space.  $\vec{\Gamma}$ 

Collisions relax distribution back to equilibrium.

$$J = \int d^3 v \, \vec{\Gamma} \cdot \frac{\partial}{\partial v} \Psi$$

N. Fisch: Current generated in parallel direction even if push is in perpendicular direction



#### **Adjoint Approach:** S. Hirshman, PoF, 23, 1238 (1980), TMA and KR Chu, PoF 25, (1982)

For a Homogeneous Plasma, we want to solve steady state kinetic

equation

$$\frac{\partial f}{\partial t} = 0 = C(f) - \frac{\partial}{\partial \mathbf{v}} \cdot \Gamma$$
Problem #1

Linearized collision operator

RF induced velocity space flux

Then find parallel current

$$J_{\parallel} = -e \int d^3 v \, v_{\parallel} f$$

#### Problem #2

Adjoint problem: Spitzer-Harm Distribution function driven by a DC electric field.

$$-ev_{\parallel}f_{M} = C(g)$$

Parallel current

$$J_{\parallel} = \int d^3 v \, \Gamma \cdot \frac{\partial}{\partial \mathbf{v}} \left( \frac{g}{f_M} \right)$$

### Toroidal Geometry Makes a Difference,

TMA and KR Chu, PoF 25, (1982)



### 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.

# 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 <u>magnet current/position</u>

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



<u>Conventional approach</u>: trial and error. Do many simulations with different anode potentials or positions select the best based on some metric measured at the exit.

### It will be shown ...



#### Hamilton's Equations *H*(*p*,*q*,*t*) Conserve Symplectic Area

$(\delta q_2(t$	), $\delta p_2(t)$ ) ( $\delta q_1(t), \delta p_1(t)$ )	$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}$ $\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}$
	perturbed orbit #1 $\frac{d\delta\mathbf{q}_{1}}{dt} = \frac{\partial^{2} H}{\partial \mathbf{p} \partial \mathbf{q}} \cdot \delta\mathbf{q}_{1} + \frac{\partial^{2} H}{\partial \mathbf{p} \partial \mathbf{p}} \cdot \delta\mathbf{p}_{1}$ $\frac{d\delta\mathbf{p}_{1}}{dt} = -\frac{\partial^{2} H}{\partial \mathbf{q} \partial \mathbf{q}} \cdot \delta\mathbf{q}_{1} - \frac{\partial^{2} H}{\partial \mathbf{q} \partial \mathbf{p}} \cdot \delta\mathbf{p}_{1}$	perturbed orbit #2 $\frac{d\delta \mathbf{q}_2}{dt} = \dots$ $\frac{d\delta \mathbf{p}_2}{dt} = -\dots$
	$\frac{d}{dt} \left( \delta \mathbf{p}_1 \cdot \delta \mathbf{q}_2 - \delta \mathbf{p}_2 \cdot \delta \mathbf{q}_1 \right) = 0$	Area conserved for

any choice of 1 and 2

#### **Reference Solution + Two Linearized Solutions**

$$\begin{aligned} & \left(\mathbf{x}_{j}, \mathbf{p}_{j}\right) \rightarrow \left(\mathbf{x}_{j}, \mathbf{p}_{j}\right) + \left(\delta \mathbf{x}_{j}, \delta \mathbf{p}_{j}\right) \\ & \rho(\mathbf{x}) \rightarrow \rho(\mathbf{x}) + \delta\rho(\mathbf{x}) \\ & \Phi(\mathbf{x}) \rightarrow \Phi(\mathbf{x}) + \delta\Phi(\mathbf{x}) \end{aligned}$$

**Two Linearized Solutions** 

 $[\delta x_{j}(t), \delta p_{j}(t)]$  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.

$$\left. \delta p_j \right|_0 = 0, \quad \delta x_j \Big|_0 = 0, \quad \delta \Phi(\mathbf{x}) \neq 0$$

Problem #2 (adjoint problem) Perturbed trajectories at exit, Unperturbed potential on boundary.

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

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

#### **Vertical Displacement of the Beam**



Predicted displacement / Calculated displacement = 0.9969

### Numerical Accuracy

Problem #1 (true problem) Change anode voltage, find change in RMS radius.

Problem #2 (adjoint problem) Perturbed trajectories at exit, Unperturbed potential on boundary.

$$\left. \boldsymbol{\delta} \hat{\boldsymbol{p}}_{j} \right|_{T} = \lambda \mathbf{x}_{\perp j},$$



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

#### AO 2.4-4: John Petillo, Serguei Ovtchinnikov, Aaron Jensen (Leidos), Philipp Borchard (Dymenso) Kyle Kuhn, Heather Shannon, Brain Beaudoin TMA. (U. Maryland) Application: 2D parallel plate sheet beam

- ► <u>Forward Case:</u> Grounded Inserts top and bottom
- <u>Direct Perturbation Case</u>: Electrode inserts on top and bottom set to  $\Delta V$  $\Delta V$  tested from 1 – 10,000 V



#### Mean Displacement: 2D parallel plate sheet beam - Manufacturing sensitivity to beam centering offset

- Results of direct vs. adjoint methods agree to within 0.20%.
- Verification: *Hamiltonian Approach* Excellent <u>first</u> successful Adjoint method to beam transport in a magnetic field.
- ► Results:
  - As the perturbed-case voltage values became small enough it easily entered the linear regime.
  - There is very a broad range of both  $\Lambda$  and  $\Delta V$  where the results are all in a linear regime.

**DYMENSO** 



Adjoint method predicted the deflection sensitivity to within 0.2%



DISTRIBUTION STATEMENT A. Approved for public release: distribution unlimited.



#### AO 2.4-2 – Optimization of TWT Design by Using Adjoint Approach A. Vlasov, T. M. Antonsen Jr., D. Chernin, I. Chernyavskiy

**Optimization of Small Signal Gain** 

Distance between gaps (two sections).

3 different goal functions

- 2 optimization parameters
- $p = L_{g1}, \ L_{g2}$
- Maximize:  $F_1(p) = \frac{1}{f_2 f_1} \int_{f_1}^{f_2} G(f) df$
- Minimize:  $F_2(p) = \frac{1}{f_2 f_{\mathrm{A}}} \oint_{\mathcal{F}_1}^{f_2} \int_{\mathcal{F}_1}^{f_2} \frac{f_2}{f_1 p} (f) \overline{G})^2 df$
- Maximize:  $F_3(p) =$



### 3D MHD Equilibria



Wendelstein 7-X Max Planck Institute for Plasma Physics (IPP) Greifswald, Germany Completed 2015

### Optimization of Stellarator Equilibria

→ Figures of Merit (FoM) - Examples

Plasma Beta, Rotational Transform, Quasi-symmetry

→ FoMs depend on boundary or coil shapes

→ Shape Gradient Sensitivity Functions gradient based optimization establish tolerances

Landreman and Paul, 2018 Nucl. Fusion 58 076023,

E. Paul, M. Landreman, TMA, J. PlasmaPhys. (2019), vol. 85, 905850207,J. Plasma Phys. (2021), vol. 87, 905870214

C. Othmer, J. Math. Industry 4, 6 (2014). **DRAG** Surface Sensitivities





Rotational transform

### Adjoint Symmetry Simplifies Calculations

Adjoint Approach to gradient calculation

> 500 X Speed – Up over direct calculation

#### **Uses VMEC & DIAGNO**

Hirshman and Whitman, 1983 Phys. Fluids 25 3553 H.J. Gardner 1990 *Nucl. Fusion* 30 1417

#### **Different Figures of Merit Possible**

Plasma pressure – beta Rotational transform Toroidal current Neoclassical radial transport -1/v regime Energetic particle drifts Quasi-symmetry Others



Surface shape sensitivity



Coil location sensitivity

### 3D MHD Toroidal Equilibrium



$$\frac{\text{In plasma}}{-\nabla p + \frac{\mathbf{J} \times \mathbf{B}}{c} = 0}$$
$$\nabla \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J}$$

Assume good flux surfaces in plas

 $\frac{\text{In vacuum}}{\nabla \times \mathbf{B}} = \frac{4\pi}{c} \mathbf{J}_{c}$ coil current Poloidal flux  $\mathbf{B} = \nabla \alpha \times \nabla \theta - \nabla \Phi_{p}(\alpha) \times \nabla \zeta$   $= \nabla \alpha \times \nabla \left(\theta - \iota(\alpha)\zeta\right)$ Toroidal Flux  $\iota(\alpha) = d\Phi_{p}(\alpha) / d\alpha$ Rotational transform

# Linear Perturbations to Equilibrium

$$\mathbf{J}_{c} \Rightarrow \mathbf{J}_{c} + \delta \mathbf{J}_{c}$$
$$\nabla p \Rightarrow \nabla p + \nabla \cdot \delta \mathbf{P}$$
$$\Phi_{p}(\alpha) \Rightarrow \Phi_{p}(\alpha) + \delta \Phi_{p}(\alpha)$$
$$\iota(\alpha) = d\Phi_{p}(\alpha) / d\alpha$$

Changes in current/shape/location of coils

Added pressure tensor

Change in poloidal flux profile

Generalized responses:

Changes in vacuum fields

Changes in magnetic field

Changes in toroidal current profile

$$\mathbf{A}_{v} \Rightarrow \mathbf{A}_{v} + \delta \mathbf{A}_{v}$$
$$\mathbf{B} \Rightarrow \mathbf{B} + \nabla \times (\xi \times \mathbf{B} - \delta \Phi_{p} \nabla \zeta)$$
$$I_{T} \Rightarrow I_{T} + \delta I_{T}(\alpha)$$
# Generalized Forces and Responses

 $\underline{O}$ 

**Responses** Vacuum fields

Plasma displacement Toroidal current profile

$$\begin{pmatrix} \delta \mathbf{A}_{V} \\ \boldsymbol{\xi} \\ d\delta I_{T} / d\alpha \end{pmatrix} =$$

$$\left(egin{array}{c} \delta \mathbf{J}_{_{C}} \ 
abla \cdot \delta \underline{P} \ \delta \Phi_{_{P}} \end{array}
ight)$$

Forces: Coil currents Pressure tensor Rotational transform

More generically, for two different perturbations

$$\delta x_i^{(1)} = \sum_j O_{ij} \, \delta F_j^{(1)} \quad \delta x_i^{(2)} = \sum_j O_{ij} \, \delta F_j^{(2)}$$

Onsager Symmetry Gives

$$\sum_{j} \left\{ \delta x_i^{(1)} \delta F_i^{(2)} - \delta x_i^{(2)} \delta F_i^{(1)} \right\} = 0$$

# Onsager Symmetry for 3D MHD Equilibria Self-adjoint MHD Force Operator

Pressure - Displacement

$$-\frac{2\pi}{c}\int_{VP}d\alpha\left(\delta I_{T}^{(2)}\frac{d}{d\alpha}\delta\Phi_{p}^{(1)}-\delta I_{T}^{(1)}\frac{d}{d\alpha}\delta\Phi_{p}^{(2)}\right)$$

Rotational transform – Toroidal current

$$+\frac{1}{4\pi}\int_{S} d^{2}x \mathbf{n} \cdot \left(\boldsymbol{\xi}^{(1)}\boldsymbol{\delta}\mathbf{B}^{(2)} \cdot \mathbf{B} - \boldsymbol{\xi}^{(2)}\boldsymbol{\delta}\mathbf{B}^{(1)} \cdot \mathbf{B}\right) = 0$$

Surface displacement

# Specify BC's & Constraints

Make this appear to be change in FoM

Pressure - Displacement

$$-\frac{2\pi}{c}\int_{VP}d\alpha\left(\delta I_{T}^{(2)}\frac{d}{d\alpha}\delta\Phi_{p}^{(1)}-\delta I_{T}^{(1)}\frac{d}{d\alpha}\delta\Phi_{p}^{(2)}\right)$$

Rotational transform – Toroidal current

$$+\frac{1}{4\pi}\int_{S} d^{2}x \mathbf{n} \cdot \left(\boldsymbol{\xi}^{(1)} \boldsymbol{\delta} \mathbf{B}^{(2)} \cdot \mathbf{B} - \boldsymbol{\xi}^{(2)} \boldsymbol{\delta} \mathbf{B}^{(1)} \cdot \mathbf{B}\right) = 0$$
  
Surface displacement

# Specify BC's & Constraints

Make this appear to be change in FoM



$$-\boldsymbol{\xi}^{(2)} \cdot \nabla \cdot \boldsymbol{\delta} \mathbf{\underline{P}}_{L}^{(1)}$$
 True Adjoint

Pressure - Displacement



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# Gradient-based optimization of 3D MHD equilibria

E. J. Paul, M. Landreman and T. Antonsen, Jr.



FIGURE 11. The magnetic field strength on (a) the initial boundary (4.14) and (b) the boundary optimized for quasi-symmetry on the axis (4.13).

### Optimization of Focusing Magnets in Accelerator Lattices *The University of Maryland Electron Ring*



UMER is a fully functional electron storage ring







magnets

Qualitative explanation: beam passes through focusing quad when it is big (strong fields). Passes through defocusing quad when it is small (weak Beam distributionfickpendsconfinanties parameters How to optin

#### **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 are proposed for cooling of hadron beams. Ya. Derbenev, Adapting optics for high-energy electron cooling, Tech. Rep. UM-HE-98-04-A (1998).

Cylindrical hadron beam cools via collisions when co-propagated with electron beam.

# 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





# More Optimization



Continuous magnetic field profiles

Variable magnet orientations

# Circular Accelerators-Periodicity



# Conclusion

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

Thank you.

# 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

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

 $\delta FoM = \int_{z_i}^{z_f} dz \left\{ \delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{Q} + \delta L^{(Y)} \mathbf{Q} \cdot \delta \mathbf{N}_{Q,B}^{(X)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{P} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{N}_{Q,B}^{(X)} L \right\}$ 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<sub>q3</sub>

-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

$$\mathbf{Q} = \begin{pmatrix} \frac{1}{2} \langle x^2 + y^2 \rangle \\ \frac{1}{2} \langle x^2 - y^2 \rangle \\ \langle xy \rangle \end{pmatrix} \mathbf{P} = \begin{pmatrix} \langle xx' + yy' \rangle \\ \langle xx' - yy' \rangle \\ \langle yx' + xy' \rangle \end{pmatrix} \mathbf{E} = \begin{pmatrix} \langle x'^2 + y'^2 \rangle \\ \langle x'^2 - y'^2 \rangle \\ 2 \langle y'x' \rangle \end{pmatrix}^{-0.15} \xrightarrow[-0.03]{-0.02}{-0.01} \xrightarrow[-0.03]{-0.02}$$

#### **Optimization – Space Charge Compensation**



# Next Step – Circular Accelerators



# Next Step – Circular Accelerators



# The Tricky Term $\frac{d\mathbf{a}}{d\tau} = -\underline{\mathbf{a}}^2 \cdot \frac{d}{d\mathbf{a}} F = -\underline{\mathbf{a}}^2 \cdot \left( \frac{\partial}{\partial \mathbf{a}} F \Big|_{W=0} + \frac{\partial}{\partial \mathbf{a}} F \Big|_X \right)$ $\frac{\partial}{\partial \mathbf{a}} F \Big|_{W=0} = \frac{\partial}{\partial \mathbf{X}} F \Big|_{\mathbf{a}} \cdot \frac{\partial \mathbf{X}}{\partial \mathbf{a}} \Big|_{W=0}$ This is the tricky term

Expand  $W'(\mathbf{X}, \mathbf{a})$  to first order

$$\frac{\partial}{\partial \mathbf{X}} W(\mathbf{X}, \mathbf{a}) = \delta \mathbf{X} \frac{\partial^2}{\partial \mathbf{X} \partial \mathbf{X}} W(\mathbf{X}, \mathbf{a}) + \delta \mathbf{a} \frac{\partial^2}{\partial \mathbf{a} \partial \mathbf{X}} W(\mathbf{X}, \mathbf{a}) = 0$$
$$\frac{\delta \mathbf{X}}{\partial \mathbf{a}} \bigg|_{W'=0} = -\frac{\partial^2}{\partial \mathbf{a} \partial \mathbf{X}} W(\mathbf{X}, \mathbf{a}) \left(\frac{\partial^2}{\partial \mathbf{X} \partial \mathbf{X}} W(\mathbf{X}, \mathbf{a})\right)^{-1}$$

Requires evaluating and inverting large matrices Constrained Optimization by Multiple, Relaxation *Adjoint with a Chaser* !

$$\frac{d}{d\tau}X = -\frac{\partial}{\partial X}W(X,a)\Big|_a$$
 The equilibrium

$$\frac{d}{d\tau} \mathbf{Y} = -\frac{\partial}{\partial \mathbf{Y}} \Big[ W(\mathbf{Y}, \mathbf{a}) + \lambda F(\mathbf{Y}, \mathbf{a}) \Big]$$
 The chaser

Parameter evolution  $\mu \frac{d}{d\tau} a = -\underline{a}^{2} \cdot \frac{\partial}{\partial a} \left[ \frac{W(Y,a) - W(X,a)}{\lambda} \right] - \underline{a}^{2} \cdot \frac{\partial}{\partial a} F(X,a)$   $\frac{\partial}{\partial a} F(X,a) \Big|_{\partial W/\partial X = 0}$ Only first derivatives required (6)

# How is it Supposed to Work $\mu > 1$ So that "a" evolves "slowly".

$$X \to X_{e}(a), \qquad 0 = -\frac{\partial}{\partial X} W(X,a) \Big|_{X_{e},a} \qquad X \text{ tends to} \\ \text{local} \\ Y \to X_{e} + \delta Y \qquad 0 = -\delta Y \cdot \frac{\partial^{2} W(Y,a)}{\partial X \partial X} \Big|_{X_{e},a} -\lambda \frac{\partial}{\partial X} \frac{\text{equilibrium}}{F(X,a)} \\ X_{e},a \qquad X \text{ tends to a slightly} \\ \text{Allow } a \text{ to change} a + \delta a \qquad A \text{ to change} a + \delta a \qquad A \text{ to change} a + \delta a \qquad B \text{ to chang$$

$$0 = -\delta X_{e} \cdot \frac{\partial^{2} W(Y,a)}{\partial X \partial X} \bigg|_{X_{e},a} - \delta a \cdot \frac{\partial^{2} W(Y,a)}{\partial a \partial X} \bigg|_{X_{e},a}$$
 The  $X$  equilibrium  

$$\lambda \delta F = \lambda \delta X_{e} \frac{\partial}{\partial X} F(X,a) \bigg|_{W'=0} = \delta a \delta Y : \frac{\partial^{2}}{\partial a \partial X} W(X,a) \bigg|_{x_{e},a} \approx \delta a \cdot \frac{\partial}{\partial a} \begin{bmatrix} \text{changes} \\ W(Y,a) - W(X,a) \end{bmatrix}_{x_{e}}$$

Constrained Optimization by Multiple, Relaxation *Adjoint with a Chaser* !

$$\frac{d}{d\tau}X = -\frac{\partial}{\partial X}W(X,a)\Big|_a$$
 The equilibrium

$$\frac{d}{d\tau} \mathbf{Y} = -\frac{\partial}{\partial \mathbf{Y}} \Big[ W(\mathbf{Y}, \mathbf{a}) + \lambda F(\mathbf{Y}, \mathbf{a}) \Big]$$
 The chaser

Parameter evolution  $\mu \frac{d}{d\tau} a = -\underline{a}^{2} \cdot \frac{\partial}{\partial a} \left[ \frac{W(Y,a) - W(X,a)}{\lambda} \right] - \underline{a}^{2} \cdot \frac{\partial}{\partial a} F(X,a)$   $\frac{\partial}{\partial a} F(X,a) \Big|_{\partial W/\partial X = 0}$ Only first derivatives required (4)

# Moment Eqs. – Circular Accelerators



# Conclusion

Adjoint method allows for optimization of Round to Flat and Flat to Round transformers.

Periodic lattices may (?) be handled by "Adjoint with a Chaser". We are currently testing using moment equations

Formalism extended to treat particle description - done

"Adjoint with a Chaser" may be extended to Stellarator optimization, with a side of ALPO<sup>©</sup>.

## Conclusion: Next Steps

**Add Magnetic field** 

sensitivity function

$$\sum_{j} I_{j} \left( \delta \hat{\mathbf{p}}_{j} \cdot \delta \mathbf{x}_{j} - \delta \mathbf{p}_{j} \cdot \delta \hat{\mathbf{x}}_{j} \right) \Big|_{T_{j}} = -q \varepsilon_{0} \int_{S} da \, \delta \Phi_{A} \, n \cdot \nabla \delta \hat{\Phi}_{S} - \mu_{0} \int d^{3} x \delta \mathbf{j}_{m} \cdot q \delta \hat{\mathbf{A}}_{S}$$
  
Change in magnetization current

Add time dependence

#### **Implement in an optimization routine**

# Basic Formulation – Linear Algebra

We wish to solve :  $\underline{A} \cdot \underline{x} = \underline{B}$  for many *B*'s.

And then evaluate for each B:  $D = \underline{C} \cdot \underline{x}^{\dagger}$  D(B) is the answer.

Instead solve for <u>y</u> once:  $\underline{A}^{\dagger} \cdot \underline{y} = \underline{C}$ 

Then:  $D = \underline{B}^{\dagger} \cdot \underline{y}$ 

#### Radial Flux driven by RF



#### **RF** Induced Transport



Jacobian Matrix - M(t) $(\delta q(t), \delta p(t))$  $\frac{d}{dt} \left( \delta \mathbf{p}_1 \cdot \delta \mathbf{q}_2 - \delta \mathbf{p}_2 \cdot \delta \mathbf{q}_1 \right) = 0$  $\begin{pmatrix} \delta \mathbf{q}(t) \\ \delta \mathbf{p}(t) \end{pmatrix} \stackrel{\text{2.1M21}}{=} \underline{\underline{M}}(t) \cdot \begin{pmatrix} \delta \mathbf{q}(0) \\ \delta \mathbf{p}(0) \end{pmatrix}$ 2N Eigenvectors and Eigenvalues of M (q(t), p(t)) $\Lambda(t) \begin{pmatrix} \delta \mathbf{q}(0) \\ \delta \mathbf{p}(0) \end{pmatrix} = \underline{\underline{M}}(t) \cdot \begin{pmatrix} \delta \mathbf{q}(0) \\ \delta \mathbf{p}(0) \end{pmatrix}$ Solutions come in N pairs-  $\Lambda_1 \Lambda_2 = 1$  $(\delta q(0), \delta p(0))$ 

> Eigenvectors from different pairs orthogonal  $(\delta \mathbf{p}_1 \cdot \delta \mathbf{q}_2 - \delta \mathbf{p}_2 \cdot \delta \mathbf{q}_1) = 0$

#### Beamstick: Gun Baseline Geometry Particle Trajectories at Actual Voltages



#### **Theoretical Study of Statistical Variations** Example of the Adjoint Method in Action

Problem: Compute the displacement of the beam in a sheet beam gun due to a small change in anode potential or a small displacement of the anode: MICHELLE Simulations of Sheet Beam Gun



The adjoint method gives us a way to compute the displacement of the beam *without* re-running MICHELLE:

 $\delta x$  = Beam centroid displacement at gun exit

 $\delta \Phi$  = Small change or error in anode or other electrode potential

 $-\boldsymbol{n} \cdot \nabla \widehat{\Phi}$ = Sensitivity (Green's) function

$$\delta x = -\frac{q}{4\pi\lambda I} \int_{S} da\mathbf{n} \cdot \delta \Phi \nabla \delta \hat{\Phi}$$



Code (Michelle) solves the following equations: Hamilton's Equations for N particles j=1,N

 $\frac{dx_{j}}{dt} = \frac{\partial H}{\partial p} \qquad \frac{dp_{j}}{dt} = -\frac{\partial H}{\partial x}$ Accumulates a charge density  $T_{i}$ 

$$\rho(\mathbf{x}) = \sum_{j} I_{j} \int_{0}^{j} dt \,\,\delta(\mathbf{x} - \mathbf{x}_{j}(t))$$

Solves Poisson Equation

$$-\nabla^2 \Phi = \rho / \varepsilon_0$$

Iterates until converged


## **Adjoint Equations**

Base caseLinear perturbation<br/>due to change inA $\frac{d}{dz}\mathbf{Q} = \mathbf{P}$ parameters $\frac{d}{dz}$  $\frac{d}{dz}\mathbf{Q} = \mathbf{P}$ parameters $\frac{d}{dz}$  $\frac{d}{dz}\mathbf{P} = \mathbf{E} + \mathbf{O} \cdot \mathbf{Q}$  $\frac{d}{dz}\delta\mathbf{Q}^{(X)} = \delta\mathbf{P}^{(X)}$  $\frac{d}{dz}$  $\frac{d}{dz}\mathbf{E} = \mathbf{O} \cdot \mathbf{P} + \mathbf{N}L$  $\frac{d}{dz}\delta\mathbf{P}^{(X)} = \delta\mathbf{E}^{(X)} + \mathbf{O} \cdot \delta\mathbf{Q}^{(X)} + \delta\mathbf{O}^{(X)} \cdot \mathbf{Q}$  $\frac{d}{dz}$  $\frac{d}{dz}L = -\mathbf{N}^{\dagger} \cdot \mathbf{Q}$  $\frac{d}{dz}\delta\mathbf{E}^{(X)} = \mathbf{O} \cdot \delta\mathbf{P}^{(X)} + \mathbf{N}\delta L^{(X)}$  $\frac{d}{dz}$  $\frac{d}{dz}\delta L^{(X)} = -\mathbf{N}^{\dagger} \cdot \delta\mathbf{Q}^{(X)} - \delta\mathbf{N}^{\dagger(X)} \cdot \mathbf{Q}$  $\frac{d}{dz}$ 

Adjoint system

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

 $(\delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{P}^{(X)} - \delta \mathbf{Q}^{(X)} \cdot \delta \mathbf{E}^{(Y)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{E}^{(X)} - \delta L^{(Y)} \delta L^{(X)} ) \Big|_{z=z_{i}}^{z=z_{i}}$  Arbitrary Changes in focusing magnets Can show  $= \int_{z_{i}}^{z_{f}} dz \Big\{ \delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{Q} + \delta L^{(Y)} \mathbf{Q} \cdot \delta \mathbf{N}_{Q,B}^{(X)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{P} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{N}_{Q,B}^{(X)} L \Big\}$  Adjoint sensitivity

## Change in Figure of Merit

 $F(\mathbf{P}, \mathbf{Q}, \mathbf{E}, L) \qquad \delta F = \delta \mathbf{P}^{(X)} \cdot \frac{\partial F}{\partial \mathbf{P}} + \delta \mathbf{Q}^{(X)} \cdot \frac{\partial F}{\partial \mathbf{Q}} + \delta \mathbf{E}^{(X)} \cdot \frac{\partial F}{\partial \mathbf{E}} + \delta L^{(X)} \frac{\partial F}{\partial L}$ Figure of Merit

$$\left( \delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{P}^{(X)} - \delta \mathbf{Q}^{(X)} \cdot \delta \mathbf{E}^{(Y)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{E}^{(X)} - \delta L^{(Y)} \delta L^{(X)} \right) \Big|_{z=z_i}^{z=z_i}$$

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

$$\left(\delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{P}^{(X)} - \delta \mathbf{Q}^{(X)} \cdot \delta \mathbf{E}^{(Y)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{E}^{(X)} - \delta L^{(Y)} \delta L^{(X)}\right)_{z=z_{i}}^{z=z_{i}}$$

$$= \int_{z_{i}}^{z_{i}} dz \left\{\delta \mathbf{P}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{Q} + \delta L^{(Y)} \mathbf{Q} \cdot \delta \mathbf{N}_{Q,B}^{(X)} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{O}_{Q,B}^{(X)} \cdot \mathbf{P} - \delta \mathbf{Q}^{(Y)} \cdot \delta \mathbf{N}_{Q,B}^{(X)} L\right\}$$
Can show
$$Adjoint sensitivity$$

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# 32 Quadrupole magnets

Qualitative explanation: beam passes through focusing quad when it is big (strong fields). Passes through defocusing quad when it is small (weak fields). Net effect is focusing.

#### Beam distribution depends on many parameters How to optimize?

## Circular Accelerators-Periodicity



#### Effective Area – Antenna Gain

