

Adjoint Approach to Optimization and Sensitivity Analysis of RF Sources*

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Motivation: Optimization of VE RF Sources

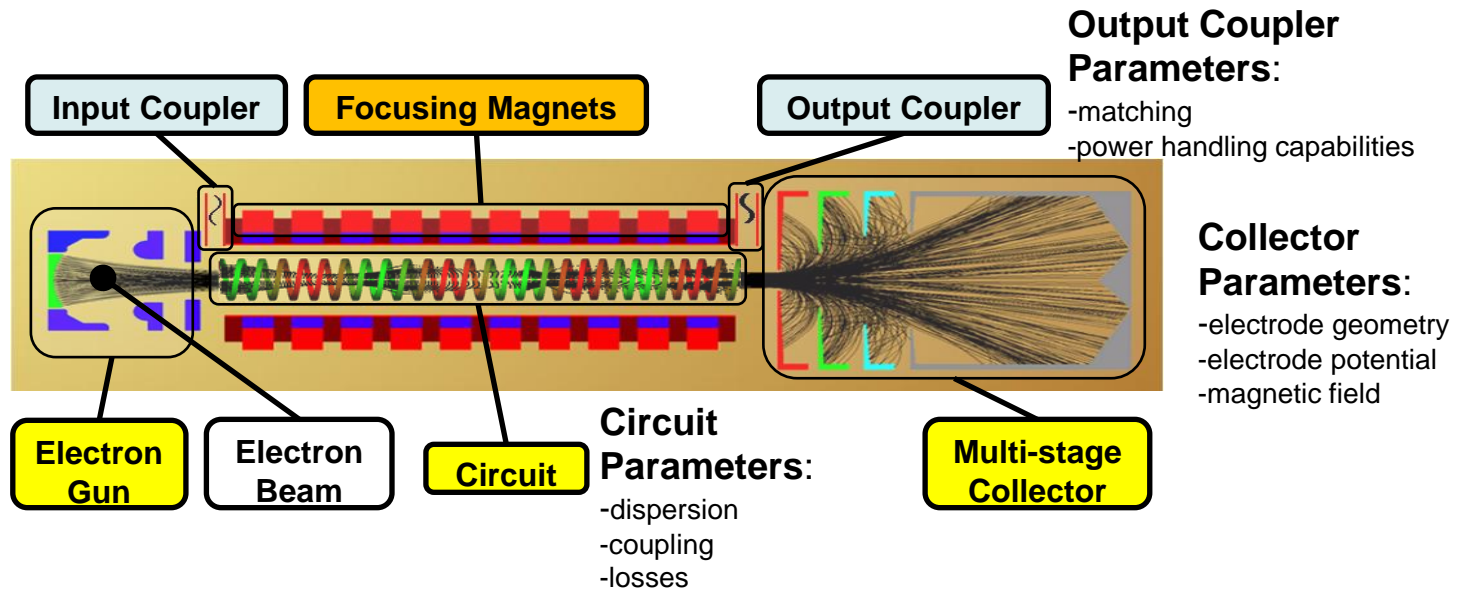
Figures of Merit (FoM):

Power
Frequency
Bandwidth
Efficiency
Size/weight

Gun Parameters:

-emission
-electrode geometry
-electrode potential
-magnetic field

Many Parameters – Computationally Intense



- Design of advanced VE RF sources requires optimization with respect to many parameters
- Accurate, geometry-driven modeling of VE devices requires substantial computational resources
- Current state-of-the-art of VE devices optimization is limited by the technical approaches and computational complexity

Key Elements of CAD Design and Optimization of RF Sources:

- Accurate, Computationally Efficient Codes
- Efficient Multi-Parameter Optimization Algorithms

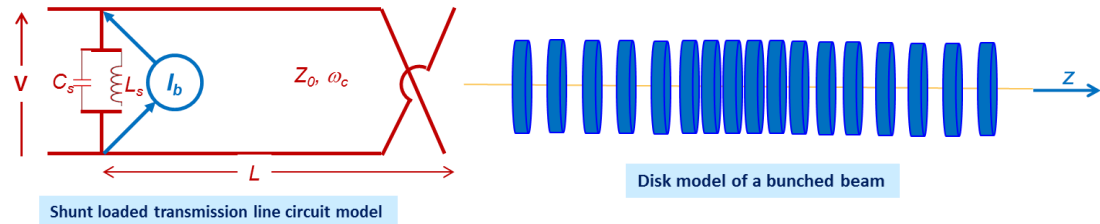
NRL/Leidos Design Codes for RF Sources

1. MAGY Gyro-devices

2. Christine 1D

- Christine Helix
- Christine CC-TWT
- Christine-FW
- Christine KL

CHRISTINE FW & Z (1D Parametric Code)



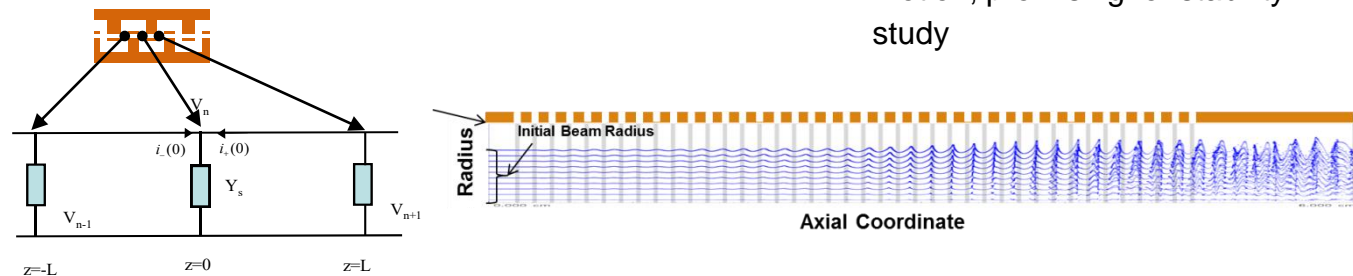
Computationally efficient, fast runs, optimization study, parametric sweep, search for optimal design, promising for stability study

3. Christine 2.5D Helix

4. TESLA 2.5D

- TESLA (Klystron)
- TESLA CC-TWT
- TESLA FW
- TESLA MBK

TESLA FW and TESLA -Z (Hybrid 2.5 D Codes)



Very accurate design tool, suitable to resolve 2D fields in beam tunnel and 3D electron motion, promising for stability study

5. TESLA-Z & Christine-Z

6. 3D PIC Code Neptune

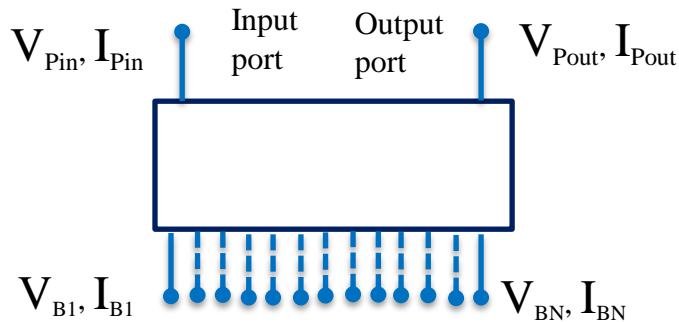
External Information on Circuit Properties as Model Parameters or Z-matrix is Needed from 3D EM Codes:

- ANSYS HFSS
- Cadence ANALYST-MP

Geometry Driven Z-Matrix Approach

Network of generalized ports:

Case with Input/Output ports & multiple-gaps



Example based on structure with 29 generalized ports (27 gaps + 2 i/o ports)

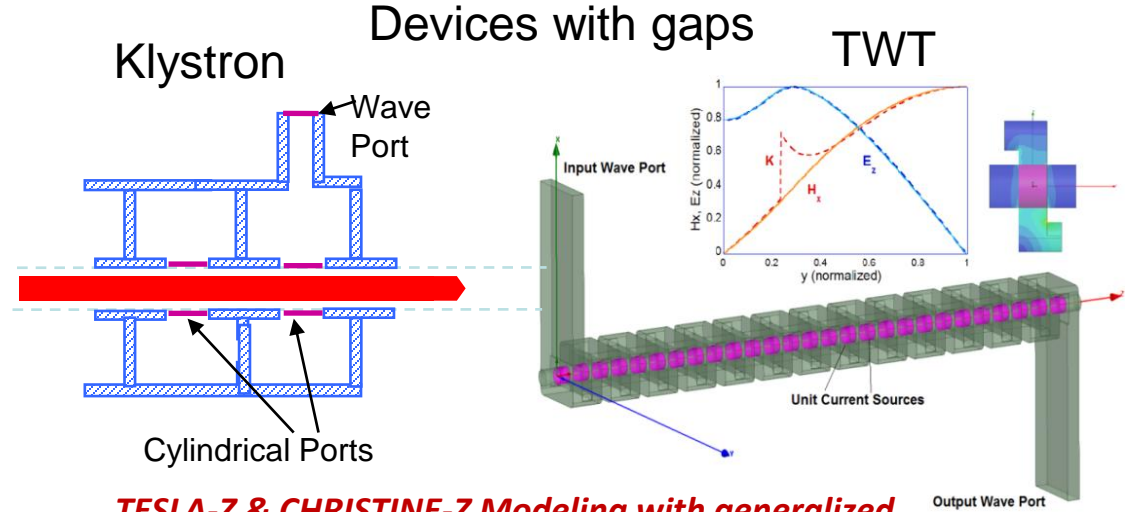
$$\begin{pmatrix} V_{Pin} \\ V_{B1} \\ V_{B2} \\ \dots \\ V_{BN} \\ V_{Pout} \end{pmatrix} = \begin{bmatrix} Z_{PinPin} & Z_{PinB_1} & Z_{PinB_2} & \dots & Z_{PinB_N} & Z_{PinPout} \\ Z_{B_1Pin} & Z_{B_1B_1} & Z_{B_1B_2} & \dots & Z_{B_1B_N} & Z_{B_1Pout} \\ Z_{B_2Pin} & Z_{B_2B_1} & Z_{B_2B_2} & \dots & Z_{B_2B_N} & Z_{B_2Pout} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ Z_{B_NPin} & Z_{B_NB_1} & Z_{B_NB_2} & \dots & Z_{B_NB_N} & Z_{B_NPout} \\ Z_{PoutPin} & Z_{PoutB_1} & Z_{PoutB_2} & \dots & Z_{PoutB_N} & Z_{PoutPout} \end{bmatrix} \times \begin{pmatrix} I_{Pin} \\ I_{B_1} \\ I_{B_2} \\ \dots \\ I_{B_N} \\ I_{Pout} \end{pmatrix}$$

$$\begin{aligned} Z_{BB} &= V_B / I_B \\ Z_{PB} &= V_P / I_B \\ Z_{BP} &= V_B / I_P \\ Z_{PP} &= V_P / I_P \end{aligned}$$

Complex matrix and vectors with voltages and currents on all ports of given structure:

$$\vec{V}(f) = \hat{Z}(f) \cdot \vec{I}(f) \quad \text{Z-matrix: 29 x 29}$$

Defined in such way Impedance matrix Z does fully characterize the frequency dependent properties and response of the given structure



TESLA-Z & CHRISTINE-Z Modeling with generalized frequency dependent response:

Large-signal codes TESLA-Z & CHRISTTINE-Z use of generalized frequency dependent impedance Z matrix¹

$$\begin{pmatrix} V_\sigma \\ V_\mu \end{pmatrix} = \hat{Z} \begin{pmatrix} I_\sigma \\ I_\mu \end{pmatrix} \longrightarrow \begin{pmatrix} I_\sigma \\ 2I_\mu^{inc} \end{pmatrix} = \hat{Y} \begin{pmatrix} V_\sigma \\ V_\mu \end{pmatrix} \quad \hat{Y} = \hat{Z}^{-1} + \hat{Y}_\mu$$

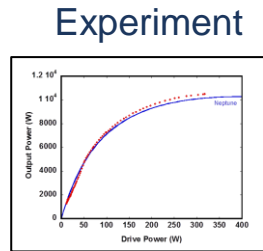
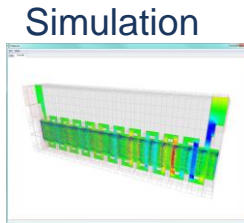
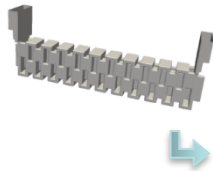
$$y_p \vec{u}_p = \hat{Y} \cdot \vec{u}_p$$

¹I.A. Chernyavskiy, T.M. Antonsen, Jr., J.C. Rodgers, A.N. Vlasov, D. Chernin and, B. Levush, "Modeling Vacuum Electronic Devices Using Generalized Impedance Matrices", IEEE TED, Vol.64, No.2, pp.536-542, Feb. 2017.

3D GPU Based PIC Code Neptune

3D Model

Sheet Beam TWT



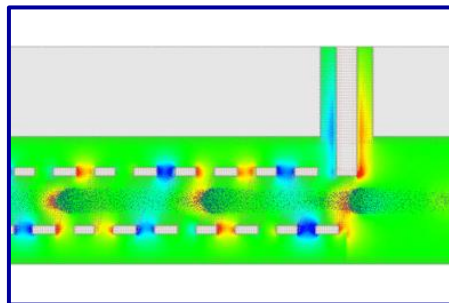
Geometry-based
3D Electromagnetic-PIC
Simulation

Neptune Fundamentals: Time Dependent Maxwell's Equations

$$\frac{\partial}{\partial t} \vec{\tilde{B}} + \vec{\nabla} \times \vec{E} = 0 \quad -\frac{\partial}{\partial t} \vec{D} + \vec{\nabla} \times \vec{\tilde{H}} = \vec{J}$$

$$\vec{\nabla} \cdot \vec{\tilde{B}} = 0 \quad \vec{\nabla} \cdot \vec{D} = \rho$$

Helix TWTA
with dielectric support
rods



- Boundary conditions:
- Second order accuracy cut-cell BC on curved boundary
 - Advanced port matching conditions

S.J. Cooke et al, ICOPS 2017

Motivation: Sensitivity of RF Sources Design

- We often need to know the sensitivity of an amplifier figure of merit F (e.g., gain, bandwidth, output power, ...) to small changes in the values of VED design parameters \vec{p} (e.g., circuit pitch profile, beam voltage, current, radius, attenuation profile ...).
- These sensitivities are expressed as derivatives, $\nabla_p F$. They are needed for:
 1. Manufacturing tolerance analysis
 2. Design optimization, using a derivative based algorithm like steepest descent.

We often have many (10's or 100's) design parameters, but just a few figures of merit or performance metrics (gain, Pout, efficiency ...) that we care about:

$$\delta F = \delta \vec{p} \cdot \nabla_p F$$

The RHS may have many terms, one for each design parameter. We need an efficient way of computing the gradient $\nabla_p F$.

Optimization Approaches at Large Scale

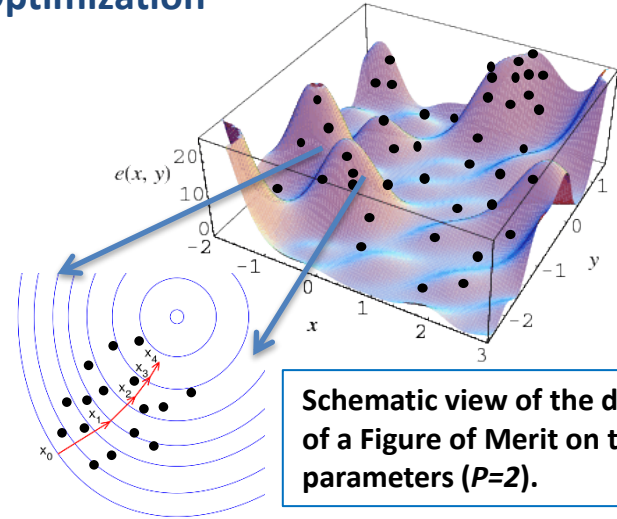
Optimization Problem



- Figure of Merit (*FoM*) or goal function (*g*)
- Parameters of Optimization



- Derivative Free Approaches
 - ✓ Runs codes to solve full size problem for many combination of parameters
 - ✓ Evaluate *FoM*
 - ✓ Select optimum
- Gradient Based Approaches
 - ✓ Calculate derivatives of *FoM* with respect to parameters
 - ✓ Move in parameter space toward optimum



Schematic view of the dependence of a Figure of Merit on two design parameters ($P=2$).

Gradient Approaches are extremely efficient for local optimization with respect to many parameters.
Key Challenge: Efficient calculation of derivatives

Adjoint approach is an example of gradient based approaches with efficient way of multi-dimensional derivative calculations. Adjoint approach demonstrated superiority with respect to other optimization approaches for multi-parameter problems, in particular for shape optimization.

Direct Approach to Calculation of $\nabla_p F$

- **Calculation of a figure of merit F usually involves a computer simulation. Some examples are:**
 - Circuit dispersion (HFSS or ANALYST)
 - Beam radius at gun exit (MICHELLE)
 - Gain*bandwidth (CHRISTINE or TESLA or NEPTUNE)

- **The most obvious way to compute $\nabla_p F$ is to run the computer simulation for each parameter of interest and approximate the derivative as a finite difference:**
 - Run 1: $p=p_0 \Rightarrow F(p_0)$
 - Run 2: $p=p_0+dp \Rightarrow F(p_0+dp)$
 - Approximate: $dF/dp \approx (F(p_0+dp)-F(p_0))/dp$

- **This ‘Direct Approach’ becomes time consuming if the number of parameters N is large:**
 - Total number of simulations = $N+1$ (ideally)
 - However, the Direct Approach may be inaccurate if dp is:
 - Too large (non-linearities)
 - Too small (roundoff)
 - As a practical matter, therefore, the need to test at least several values of dp means that the number of simulations required may be $\sim m*N+1$, where $m \gtrsim 3-5$.

Alternative: Adjoint Approach

Circuit/network theory

- ✓ S.W. Director and R.A. Rohrer, IEEE Trans. Circuit Theory (1969)

Electromagnetic analysis

- ✓ N.K. Nikolova, et al. IEEE Trans. MTT (2004)
- ✓ HFSS computation of adjoint derivatives

Fluid dynamics

- ✓ A. Jameson, Computational Fluid Dynamics Review (1995)
- ✓ C. Othmer, Journal of Mathematics in Industry (2014)

Meteorology

- ✓ R.M. Errico, Bulletin Am Met. Soc. (1997) [review]

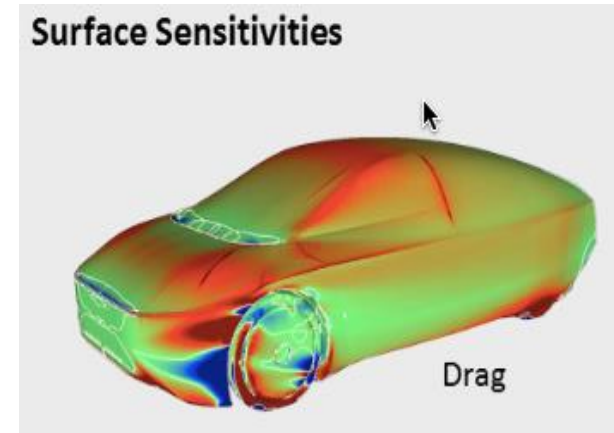
Plasma Physics

- ✓ T. M. Antonsen, Jr. and K.R. Chu, PoF 25, (1982)

Beam Optics

- ✓ T. M. Antonsen, Jr. and J.J. Petillo PoP 26, (2019)

Example: Calculating the Sensitivity Functions Over an Entire Surface
C. Othmer, Journal of Mathematics in Industry (2014)



Adjoint methods have been applied in many fields and demonstrated superiority with respect to other optimization approaches for multi-parameter problems, in particular for shape optimization.

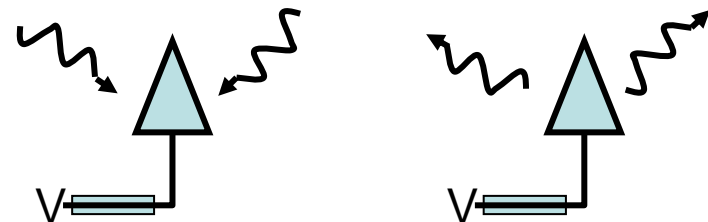
Application of adjoint techniques to particular problem requires unique theoretical work on formulation of adjoint problem.

Adjoint Approach for Particles Dynamic

- Shot noise on gyrotron beams, **T.M. Antonsen, Jr.**, W. Manheimer and A. Fliflet, PoP (2001).
- Beam optics sensitivity function, **T.M. Antonsen, Jr.**, D. Chernin, J. Petillo, Phys. Plasmas 26, 013109 (2019);
- Stellarator Optimization and Sensitivity, E. Paul, M. Landreman, T.M. Antonsen, Jr., *J. Plasma Phys.* (2019), vol. 85, 905850207, *J. Plasma Phys.* (2021), vol. 87, 905870214
- Optimization of Flat to Round Transformers in Particle Accelerators, L. Dovlatyan, B. Beaudoin, S. Bernal, I. Haber, D. Sutter and **T.M. Antonsen, Jr.**, Phys Rev Accel and Beams V25, 044002 (2022).
- Adjoint Equations for Beam-Wave Interaction and Optimization of TWT Design, A. Vlasov, **T.M. Antonsen, Jr.**, D. Chernin and I. Chernyavskiy, IEEE Trans. Plasma Sci. V. March (2022).

Adjoint Approach in VE Related Fields

- An *Adjoint Method* is a technique based on a reciprocity principle, which facilitates the computation of the effects of small changes of design parameters on selected figures of merit.



Example of reciprocity:
Antenna receiving pattern =
Antenna transmitting pattern

- We have previously developed adjoint methods for the evaluation of the effects of (1) small changes in geometry in an electron gun and small changes in beam voltage, current, gap spacing profiles in a FWG TWT(2), Helix TWT(3).
 - 1) T.M. Antonsen, Jr., D. Chernin, and J.J. Petillo, “Adjoint approach to beam optics sensitivity based on Hamiltonian particle dynamics,” *Phys. Plasmas* 26, 013109 (2019).
 - 2) A.N. Vlasov, T.M. Antonsen, Jr., D. Chernin, and I.A. Chernyavskiy, “Adjoint Equations for Beam-Wave Interaction and Optimization of TWT Design,” *IEEE Trans. Plasma Sci* 50 2568-2577 (2022).
 - 3) D. Chernin, A.N. Vlasov, T.M. Antonsen, Jr., and I.A. Chernyavskiy, “Adjoint Equations and Their Application to Helix TWT Design,” *IEEE Trans. Electron Devices* (Early Access) (June 2024).

Application of the adjoint method requires only 3 runs of a simulation code to compute all N partial derivatives, compared with (at least) $N+1$ runs for the ‘Direct Method’ !!

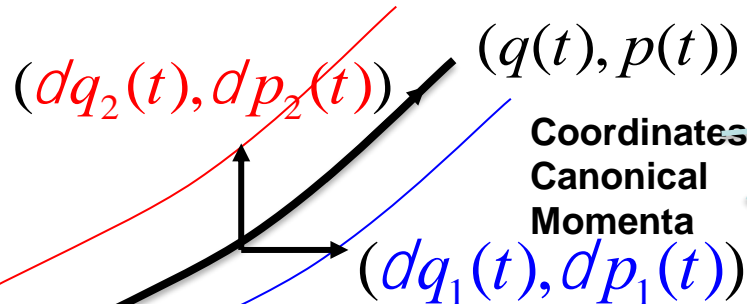
Fundamentals of Adjoint Approach to Beam-Wave Interaction

Symplectic Area Conservation Law for particles interacting with EM fields:

- Works explicitly for Hamilton's Equations
- Works implicitly for other forms of particles- field equations

Symplectic Area conserved for any choice of perturbed trajectories 1 and 2

$$\frac{d}{dt} (d\mathbf{p}_1 \times d\mathbf{q}_2 - d\mathbf{p}_2 \times d\mathbf{q}_1) = 0$$



Hamilton's Equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

Perturbed orbit #1

Perturbed orbit #2

$$\frac{dd\mathbf{q}_1}{dt} = \frac{\partial^2 H}{\partial \mathbf{p} \partial \mathbf{q}} \times d\mathbf{q}_1 + \frac{\partial^2 H}{\partial \mathbf{p} \partial \mathbf{p}} \times d\mathbf{p}_1$$

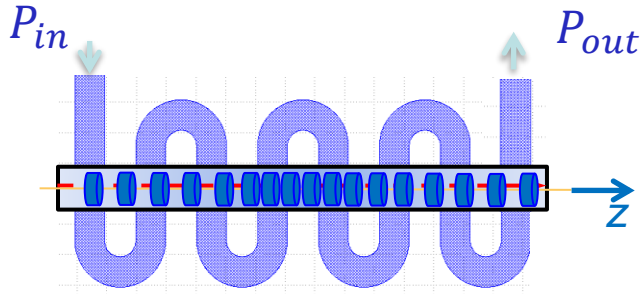
$$\frac{dd\mathbf{p}_1}{dt} = -\frac{\partial^2 H}{\partial \mathbf{q} \partial \mathbf{q}} \times d\mathbf{q}_1 - \frac{\partial^2 H}{\partial \mathbf{q} \partial \mathbf{p}} \times d\mathbf{p}_1$$

$$\frac{dd\mathbf{q}_2}{dt} = \dots$$

$$\frac{dd\mathbf{p}_2}{dt} = -\dots$$

Beam-Wave Interaction in 1D Approximation

Folded Waveguide TWT



Implemented in Christine-Z Code

- RF fields at input frequency + temporal harmonics
- 1D Equations of Electron Motion + Disk Model for Space Charge Fields

- Bunched Beam Effect
- Use Z-matrices for circuit field calculation

$$I_n = I_b \int dz e_n^*(z - z_n) \langle e^{i\omega t_i(z)} \rangle$$

$$V_n = \sum_{n'=1,N} Z_{nn'} I_{n'} + 2 \sum_{n'=N+1,P} Z_{nn'} I_{n'}^+$$

1D Equations of Motion can be expressed in Hamiltonian Form

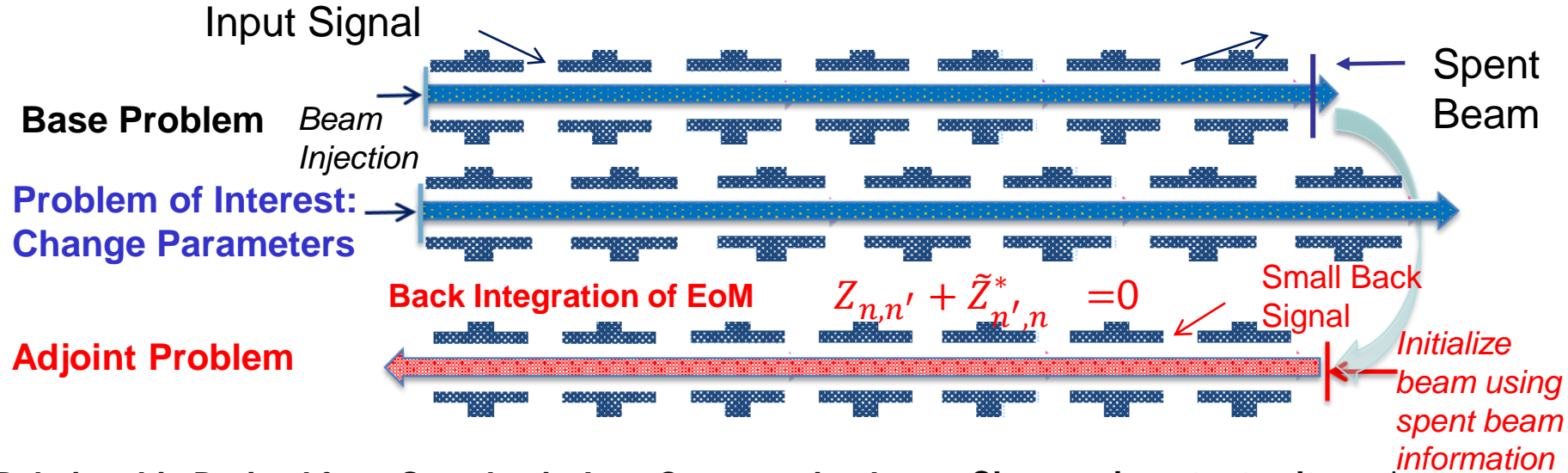
$$P(E_i, t_i; z) = m\gamma v_z(E_i) - \sum_n \left[\frac{iqV_n e_n(z)}{\omega} e^{-i\omega t_i} + c.c. \right] - \left[\frac{qE_0}{\omega} e^{-i\omega t_i} \langle e^{i\omega t_i} \rangle + c.c. \right]$$

$$\frac{dE_i}{dz} = - \frac{\partial}{\partial t_i} P(E_i, t_i; z).$$

$$\frac{dt_i}{dz} = \frac{\partial}{\partial E_i} P(E_i, t_i; z).$$

1. A.N. Vlasov, T.M. Antonsen, D. Chernin, I.A. Chernyavskiy, "Adjoint Equations for Beam-Wave Interaction and Optimization of TWT Design," IEEE Trans. on Plasma Science, IEEE Trans. Plasma Sci 50 2568-2577 (2022).
2. I.A. Chernyavskiy, T.M. Antonsen, Jr., J.C. Rodgers, A.N. Vlasov, D. Chernin and B. Levush," Modeling Vacuum Electronic Devices Using Generalized Impedance Matrices," IEEE Trans. Electr. Dev., vol 64, pp. 536-542, Feb 2017,

Adjoint Approach for 1D Beam-Wave Interaction



Relationship Derived from Symplectic Area Conservation Law **Changes in output voltage due to:**

$$-2 \sum_{n=N+1,P} \left[dI_n^{Y*+} dV_n^X - c.c \right] = \frac{W}{iq} \frac{I}{N} \sum_i \left(dt_i^Y dE_i^X - dt_i^X dE_i^Y \right) \Big|_0$$

$$- \sum_{\substack{n=1,P \\ n'=1,P}} \left[\left(dI_n^{Y*}, 2dI_n^{Y*+} \right) dZ_{mn'} \left(I_{n'}, 2I_{n'}^+ \right) - c.c \right] + I \int_0^L dz \left[\left(dy^{Y*} V_n + y^* dV_n^Y \right) de_n(z) - c.c \right]$$

- Variations in particles energy
- Variations in pre-bunching
- Variations in gap position and shape
- Variations in circuit parameters

Using the Adjoint Relationship we can find multi-dimensional derivatives without multiple solutions of the beam-wave interaction problem:

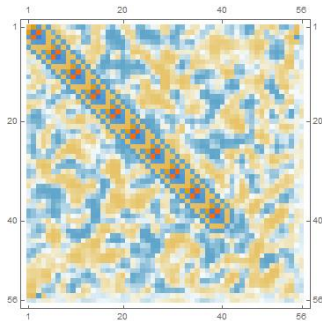
- Solution of base problem (known, one run of the code was needed)
- **Solution of Adjoint problem (known, two runs of the code was needed)**
- **Derivatives for variations of our interest now can be found as sums or integrals without repetitive code runs**

Circuit Parameters Variations Term in Adjoint Relationship

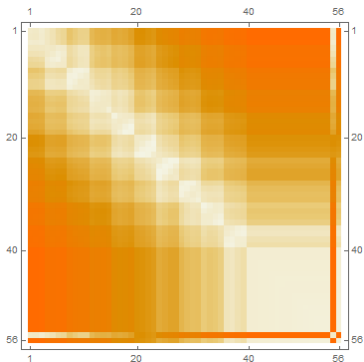
$$\sum_{\substack{n=1,P \\ n'=1,P}} [\delta V_n^{Y*} \delta Y_{n,n'} V_{n'} - c. c.]$$

3D EM calculations

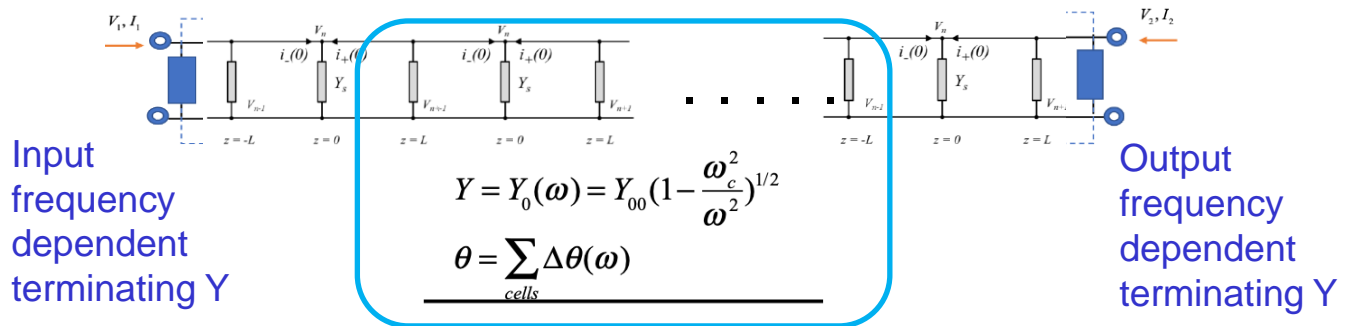
δY matrix structure



δZ matrix structure



Evaluation of Local Multi Parameter Variations By N Cells Transmission Line Model



N cells based on line-shunt model to calculate δY matrix (properties of each individual cell might be varied)

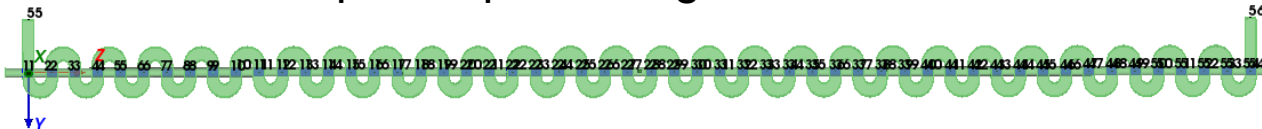
Unit cell parameters are fitted using calculated dispersion curve

Optimization Using Adjoint Method

- We are developing a general purpose design optimization capability for TWTs, based on the adjoint method.
 - By “optimization” we mean finding a maximum or minimum of a scalar figure of merit as a function $F(\vec{p})$ of a set of design parameters \vec{p} .
 - $F(\vec{p})$ is usually computed by running a large signal TWT code like CHRISTINE-Z.

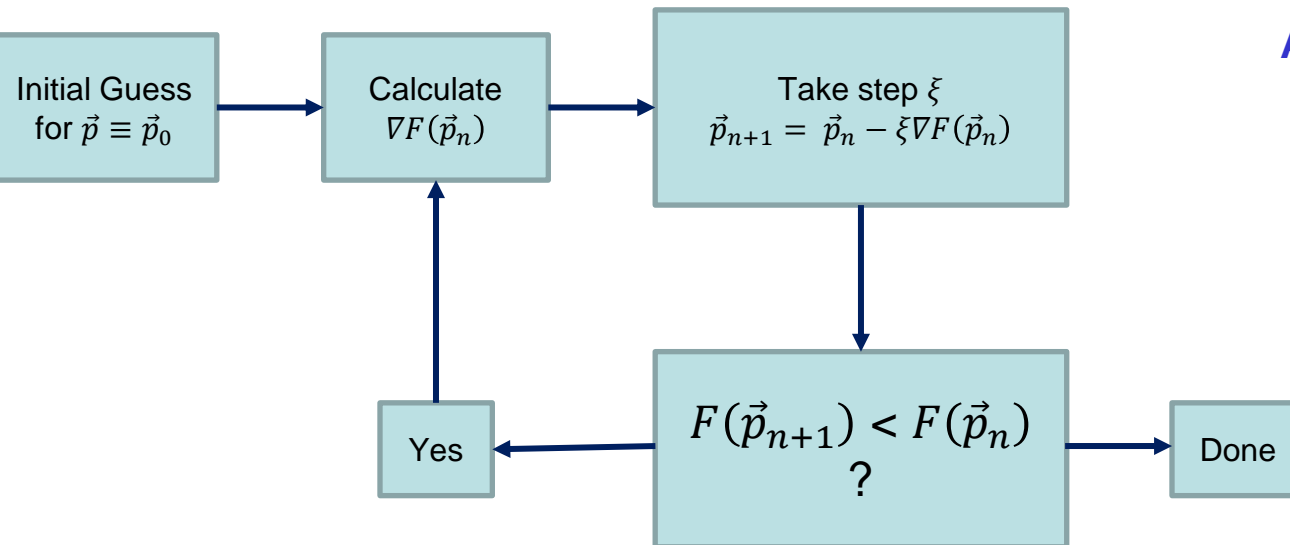
- The adjoint method may be used to compute the partial derivatives of $F(\vec{p})$, with respect to the design parameters.
 - The adjoint method requires just 2 specially designed runs of a large signal code like CHRISTINE-Z, to compute $\nabla F(\vec{p})$, independent of the dimension of \vec{p} !
 - These partial derivatives may be used in a derivative-based optimizer, e.g., steepest descent

TWT with uniform 54 gaps hybrid serpentine structure connected to input/output waveguides: 20 kV beam



A.N. Vlasov, T.M. Antonsen, D. Chernin, I.A. Chernyavskiy, “Adjoint Equations for Beam-Wave Interaction and Optimization of TWT Design,” IEEE Trans. on Plasma Science, v. 50, pp.2568-2577 June 2022.

- Find minimum of $F(\vec{p})$ using steepest Descent Algorithm:



Average Gain over Bandwidth

$$\langle g \rangle \equiv \frac{1}{(f_2 - f_1)} \int_{f_1}^{f_2} g(f) df$$

Gain Flatness

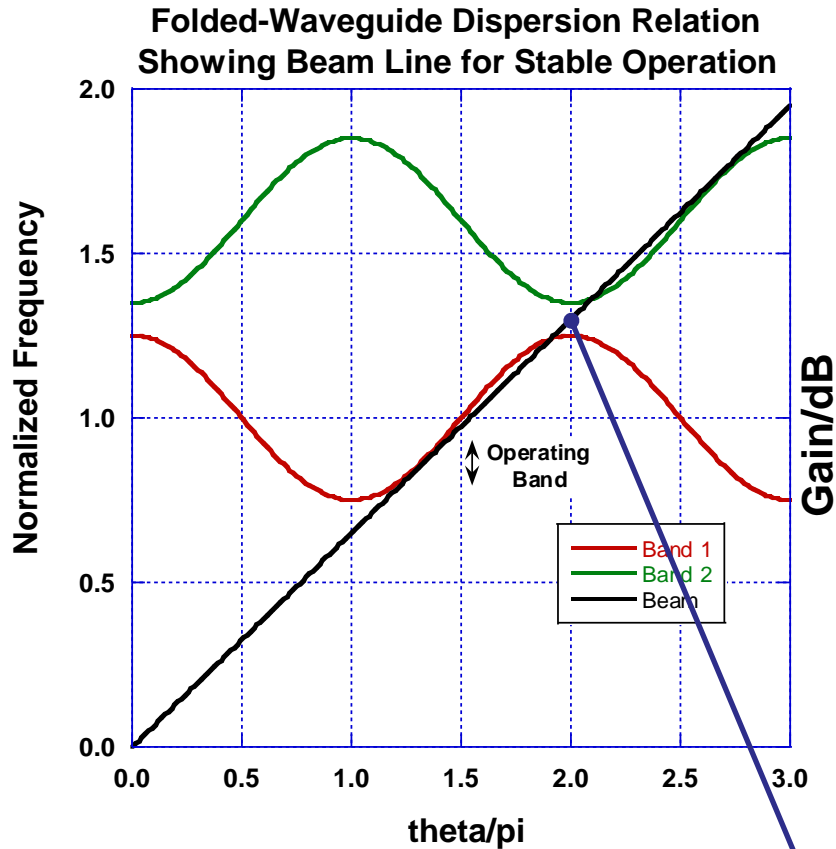
$$\sigma_g^2 \equiv \frac{1}{(f_2 - f_1)} \int_{f_1}^{f_2} (g(f) - \langle g \rangle)^2 df$$

Gain * Bandwidth Product

$$\Gamma_p \equiv \frac{\langle g \rangle}{\sigma_g^p}$$

- Each calculation of $F(\vec{p})$ requires 1 runs of CHRISTINE-Z
- Each calculation of $\nabla F(\vec{p}_n)$ requires 2 runs of CHRISTINE-Z

Constrained Optimization: Optimize Circuit Pitch

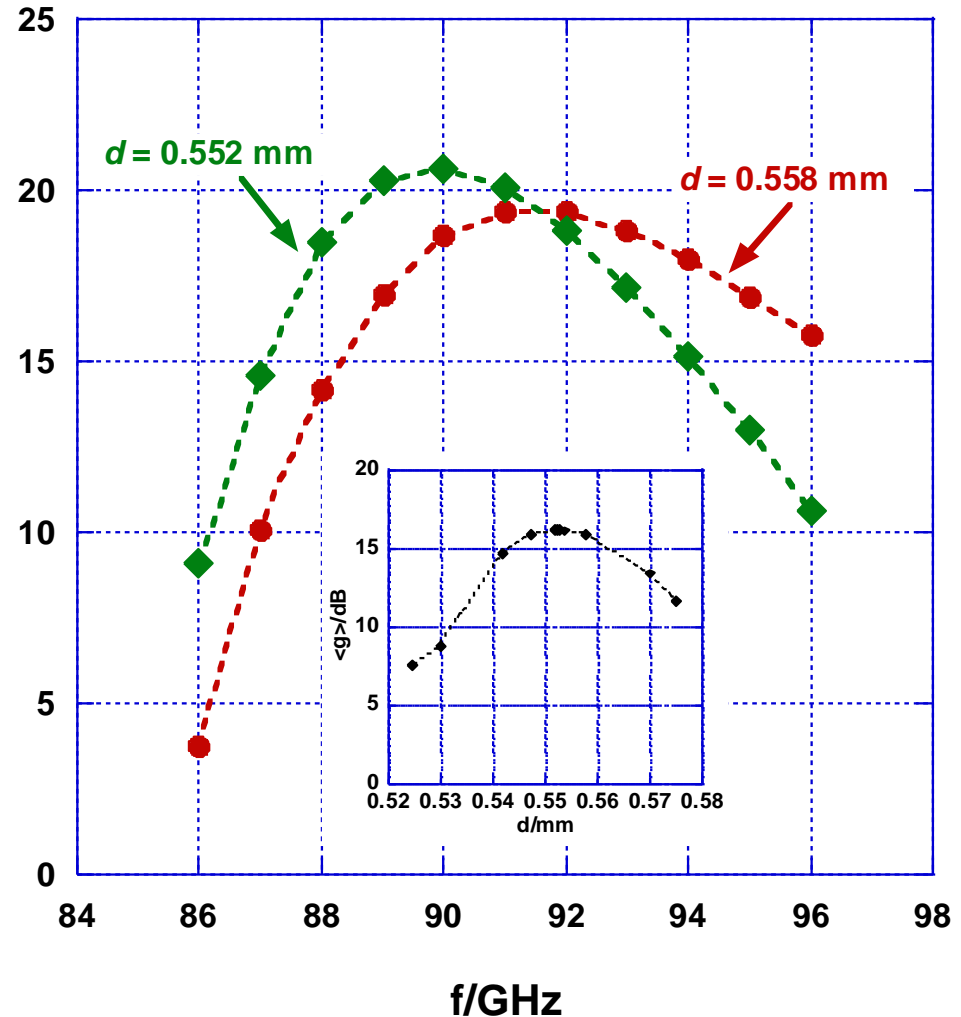


■ $p = L_g$

■ Maximize: $F_1(p) = \frac{1}{f_2 - f_1} \int_{f_1}^{f_2} G(f) df$

– Ensures that the beam line passes through the band gap at 2π .

- Avoids backward wave and band edge oscillations.



Optimization of Two Section TWT

Optimization of Small Signal Gain

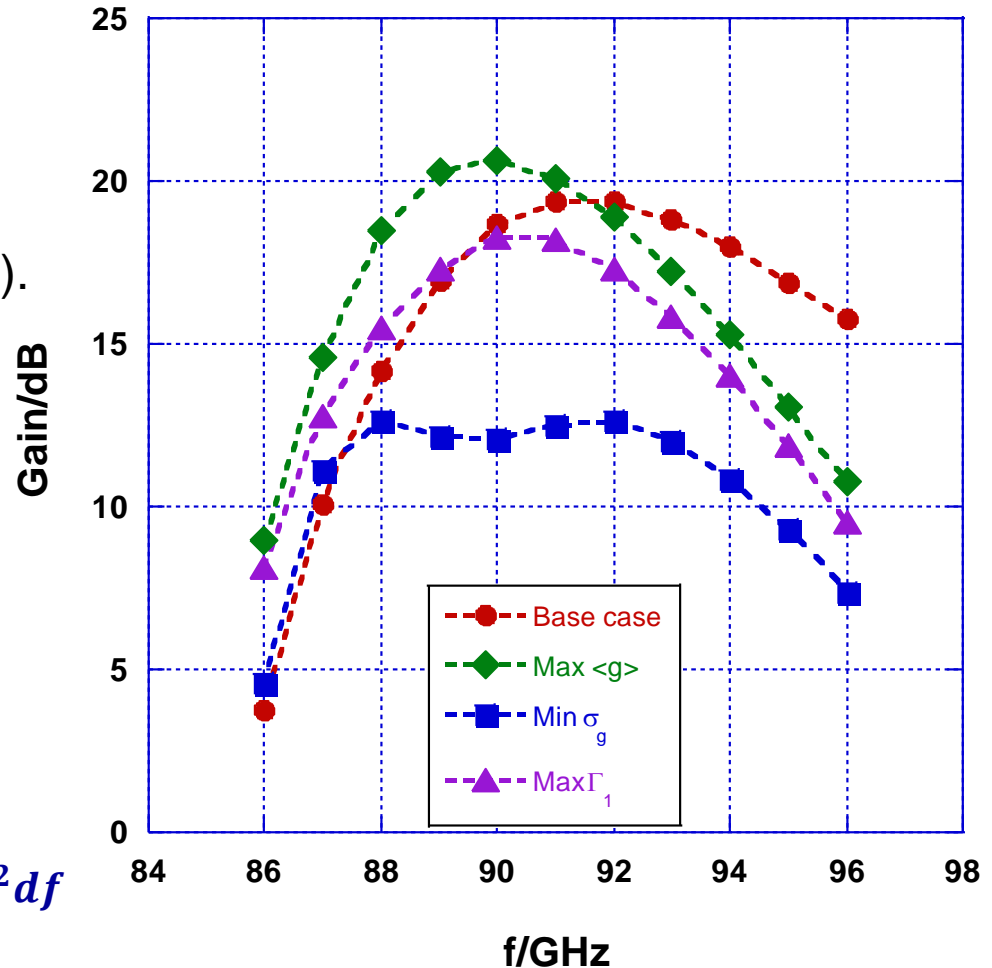
Distance between gaps (two sections).
3 different goal functions
2 optimization parameters

■ $p = L_{g1}, L_{g2}$

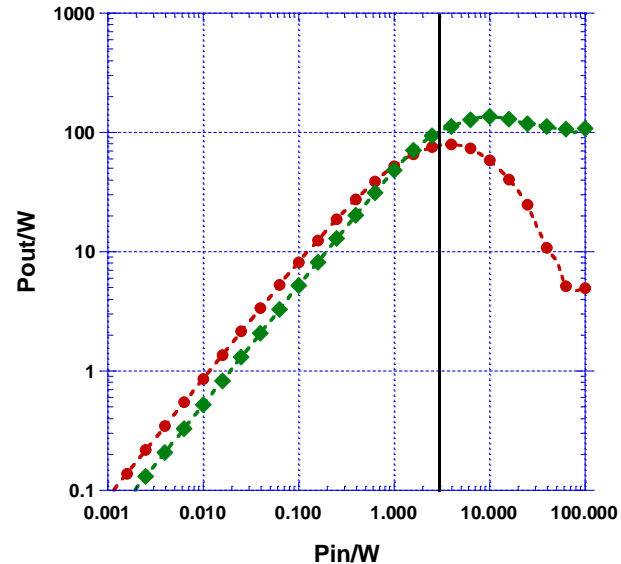
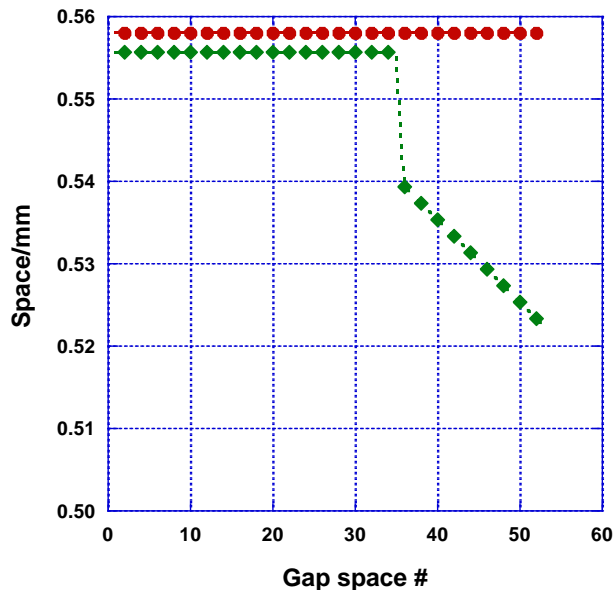
■ **Maximize:** $F_1(p) = \frac{1}{f_2 - f_1} \int_{f_1}^{f_2} G(f) df$

■ **Minimize:** $F_2(p) = \frac{1}{f_2 - f_1} \int_{f_1}^{f_2} (G(f) - \bar{G})^2 df$

■ **Maximize:** $F_3(p) = \Gamma_p \equiv \frac{\langle g \rangle}{\sigma_g^p}$

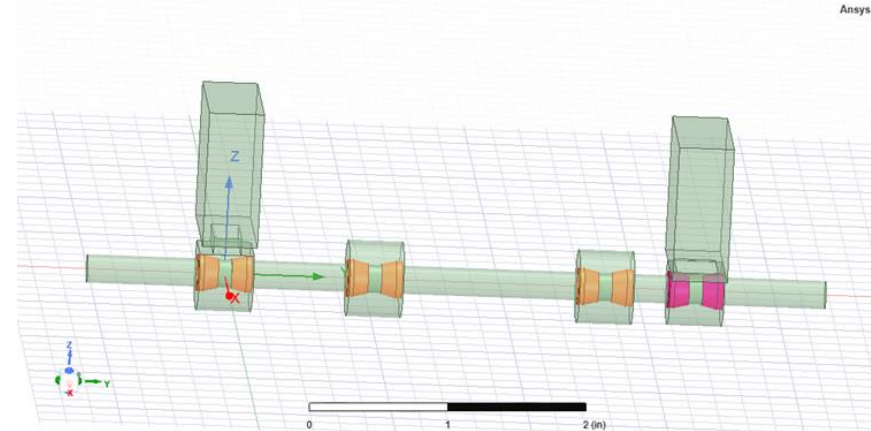


Example: Find Circuit Pitch Profile to Maximize Output Power at a Single Frequency (91 GHz)

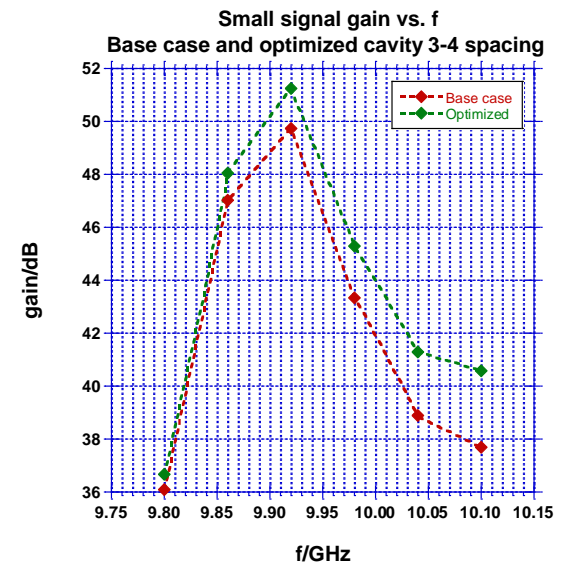


- **3 parameter optimization**
 - flat pitch section (1 parameter) + linear ramp section (2 parameters)
 - Pin = 3W fixed
- Base case: Flat pitch profile, Pout(91 GHz) = 77.9 W
- **Result of optimization: Pout(91 GHz) = 101.1 W (+1.1 dB)**
 - Peak output power increased from 79.3 W to 136 W (+2.3 dB)

- CPI 4-cavity X-band klystron*
 - Fixed cavity properties (Z-matrix)
 - Variable beam voltage, cavity spacings
 - Base case parameters:
 - $V_b = 115$ kV
 - $I_b = 78.1$ A
 - $r_b = 0.152$ cm
 - Cavity spacings:
 - » 1-2: 2.776 cm
 - » 2-3: 4.265 cm
 - » 3-4: 1.676 cm

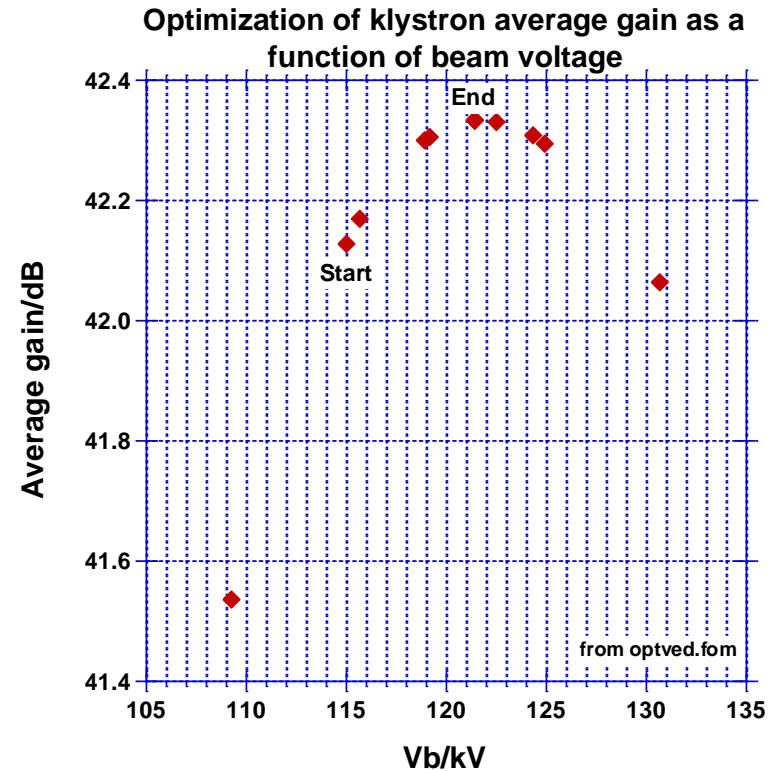
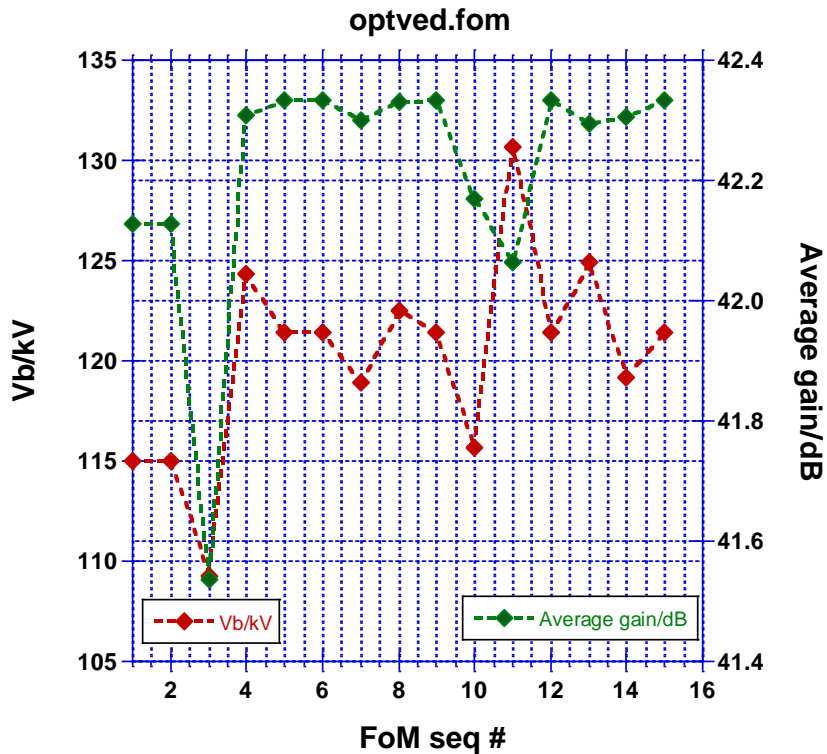


- Example: Maximize average small signal gain across band
 - 6 equally spaced frequencies in [9.8-10.1] GHz



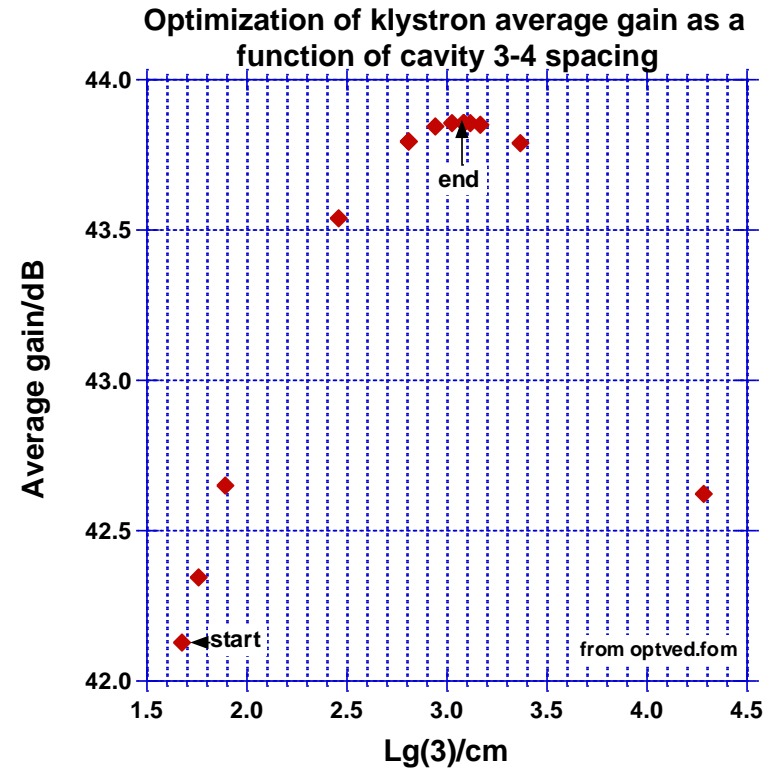
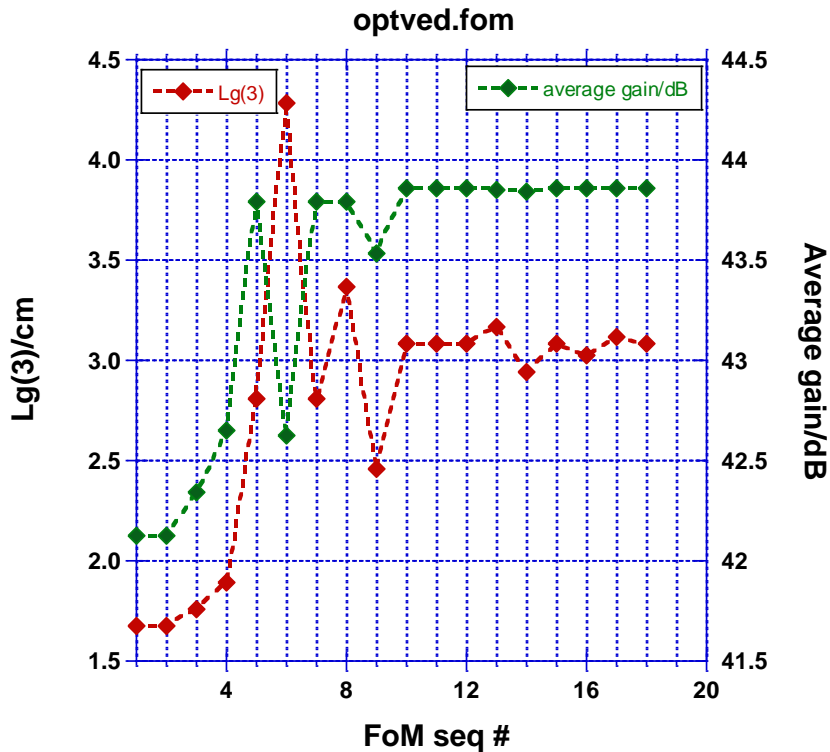
*Courtesy of R. Begum, CPI

Klystron Optimization

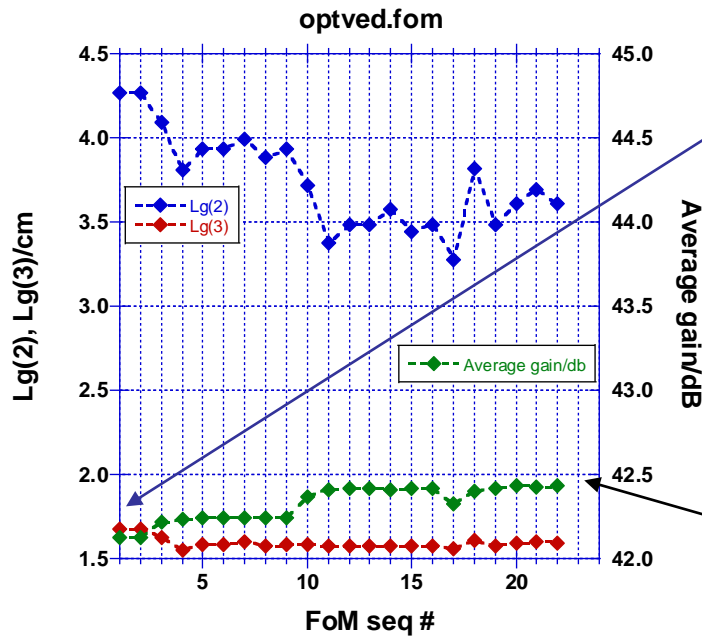


- Result: Increase in average gain by ~0.2 dB by increasing beam voltage by ~ 6.4 kV (5.6%).

Klystron Optimization of Spacing Between Cavities

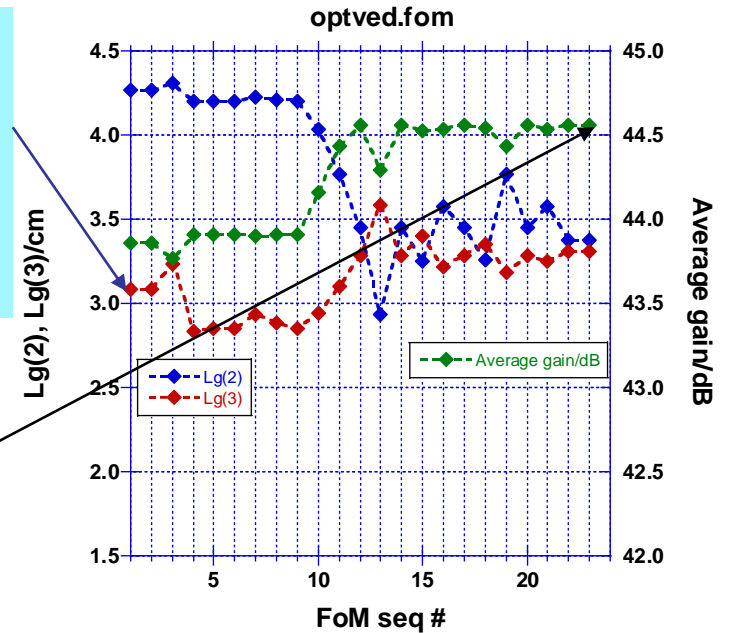


- Result: Increase in average gain by ~1.7 dB by increasing cavity 3-4 spacing by ~ 1.4 cm (84%).

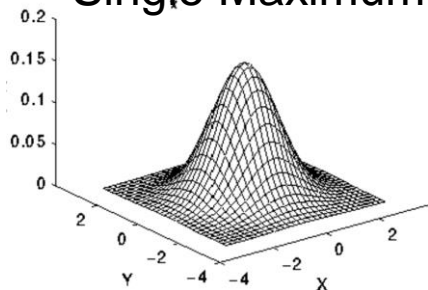


Different Initial Set of Parameters of Optimization

Different Optimal Solutions

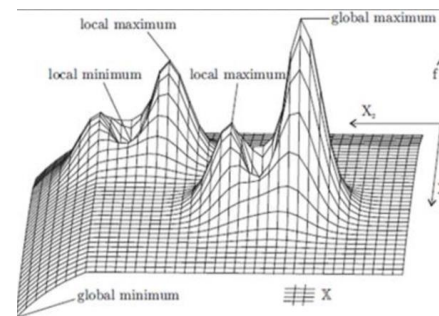


Single Maximum



More Realistic Case for VED

Several Local Maxima



Summary/Ongoing Work

- **Adjoint methods are a powerful way to evaluate parameter dependences in many RF Sources based on self-consistent beam-wave interaction.**

- **An adjoint method for the evaluation of the sensitivity of the performance of a FW TWT and Klystron to small changes in various design parameters has been formulated and implemented in the CHRISTINE-1D large signal code.**

- **The method has been successfully tested against direct calculation of changes in gain and output power due to changes in various design parameters, including beam voltage, beam current, circuit phase velocity and circuit impedance.**

- **Our recent and planned work include development and implementation of the adjoint method for:**
 - **Multi-parameter optimization for large signal case for klystron**
 - **Algorithms for Case with large number of design parameters**
 - **2D large signal simulations (TESLA-Z code)**