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A fast 1D charge-conserving particle-in-cell code for the modeling of klystrons

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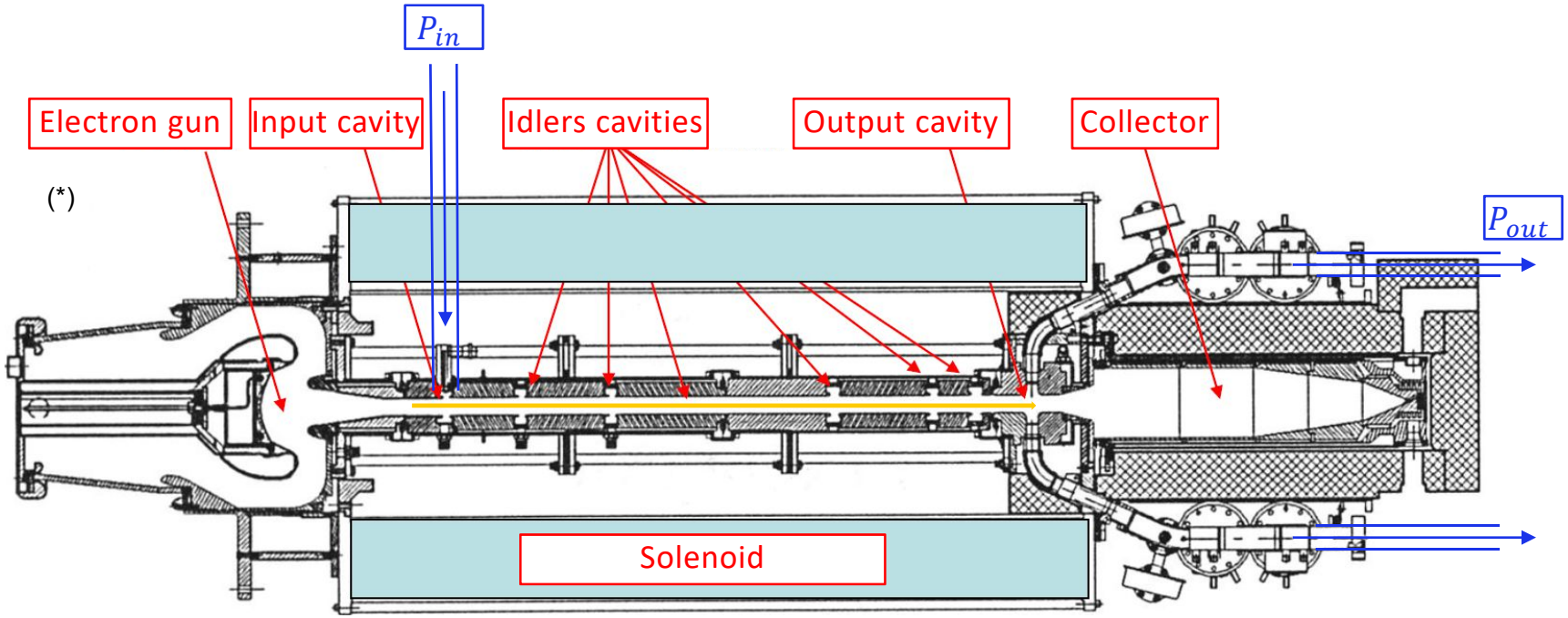
Klystrons - Overview



Typical arrangement of a high-power klystron

(*) Adapted from Sprehn D. et al, Performance of a 150-MW S-Band Klystron, AIP. Conf. Proc. 337, 1995, p. 44

Distribution function and Vlasov equation

- Electrons emitted from the gun are characterized by a 7D distribution function $f(\mathbf{x}, \mathbf{p}, t)$ that corresponds to a statistical mean of repartition of e- in phase space

- Properties:

  - Electronic density given by $n(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{p}, t)\, d^3p$

  - Mean velocity $\mathbf{v}(\mathbf{x}, t)$ verifies $n(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t) = \int \mathbf{v} f(\mathbf{x}, \mathbf{p}, t)\, d^3p$

  - Distribution function evolves according to the relativistic Vlasov equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_{\mathbf{x}} f - e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{p}} f = 0 \quad \text{with:} \quad \mathbf{v} = \frac{\mathbf{p}}{m_o \gamma}$$

  - Charge and current densities, $\rho(\mathbf{x}, t) = -en(\mathbf{x}, t)$ and $\mathbf{J}(\mathbf{x}, t) = -en(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t)$, sources terms for Maxwell's equations

Macroparticles and reduction to 1D

- Approximation of the distribution function for n_p point-charge macroparticles:

$$f_{n_p}(\mathbf{x},t) = w\sum_{i=1}^{n_p}\delta\big(\mathbf{x}-\mathbf{x}_i(t)\big)\delta\big(\mathbf{p}-\mathbf{p}_i(t)\big)$$

  where w is the number of e- per macroparticle

- With the macroparticles charge $q_p = -ew$, the particle density and the charge and current densities and current are then:

$$n_{n_p}(\mathbf{x},t) = w\sum_{i=1}^{n_p}\delta(\mathbf{x}-\mathbf{x}_i(t)) \qquad \rho_{n_p}(\mathbf{x},t) = q_p\sum_{i=1}^{n_p}\delta(\mathbf{x}-\mathbf{x}_i(t))$$

$$\mathbf{J}_{n_p}(\mathbf{x},t) = q_p\sum_{i=1}^{n_p}\mathbf{v}(t)\delta(\mathbf{x}-\mathbf{x}_i(t))$$

- Define linear charge and current densities:

$$\rho_{z,n_p}(z,t) = q_p\sum_{i=1}^{n_p}\delta(z-z_i(t)) \qquad J_{z,n_p}(z,t) = q_p\sum_{i=1}^{n_p}v_{z,i}(t)\delta\big(z-z_i(t)\big)$$

Macroparticles equations of motion

- Model assumptions:
  - Electron flow confined to longitudinal direction by infinite longitudinal focusing magnetic field propagating along drift tube of radius a
    i.e. neglects any transverse motion
  - Beam current I_0 low enough to neglect beam self-magnetic field
  - Beam radius b constant along the longitudinal direction

- Taking the moments of the relativistic Vlasov equation with the approximated distribution function, it can be shown that the motion of the macroparticles is ruled by the equations of motion:

$$\frac{dz_i}{dt} = v_{z,i} \text{ and } \frac{d(\gamma v_z)_i}{dt} = \frac{q_p}{m_p}\left(E_{z,rf}(z_i(t)) + E_{z,sc}(z_i(t))\right)$$

$E_{z,rf}$ corresponds to the rf cavity fields,
$E_{z,sc}$ is the averaged space-charge field induced by all macroparticles
m_p, mass of a macroparticle such that: $\frac{q_p}{m_p} = \frac{e}{m_0}$

Normalizations, particles charge and RF e-field

- Unbunched e- beam propagates at the velocity v_o and RF signal to be amplified has frequency f.
- Normalization of distances to $\lambda_e = \frac{v_o}{f}$ i.e. new longitudinal coordinate: $y = \frac{z}{\lambda_e}$
- Normalization of times to RF period $\tau = tf$
- Define particles charge by: $q_p = -\frac{I_0}{n_{p0,cycl} f}$ where $n_{p0,cycl}$ is the number of particles per RF cycle when there is no bunching and I_0 is the beam current
- Normalization of the velocities to v_o: $u_i = \frac{v_{z,i}}{v_0}$
- Normalization of the nth RF cavity e-fields: $E_{z,rf,n}(y,\tau) = v_n(\tau) e_n(y)$ where v_n is the cavity n instantaneous voltage normalized to the depressed gun voltage V_0 and e_n is the normalized cavity profile along the axis i.e.: $\int_{-\infty}^{+\infty} e_n(y) dy = 1$

Normalizations and space-charge e-field

- Normalization of the linear electronic density: $n_{y,n_p}(y,\tau) = w \sum_{i=1}^{n_p} \delta(y - y_i(\tau))$

- Normalization of the linear charge density: $\rho_{y,n_p}(y,\tau) = q_p \sum_{i=1}^{n_p} \delta(y - y_i(\tau))$

- Normalization of the current density: $J_{y,n_p}(y,\tau) = q_p \sum_{i=1}^{n_p} u_i(\tau)\delta(y - y_i(\tau))$

- Knowing the Green's function $G_{y,\rho}$ of a unit-charged source disk of radius b confined in a cylindrical tube of radius a, the normalized space-charge e-field is:

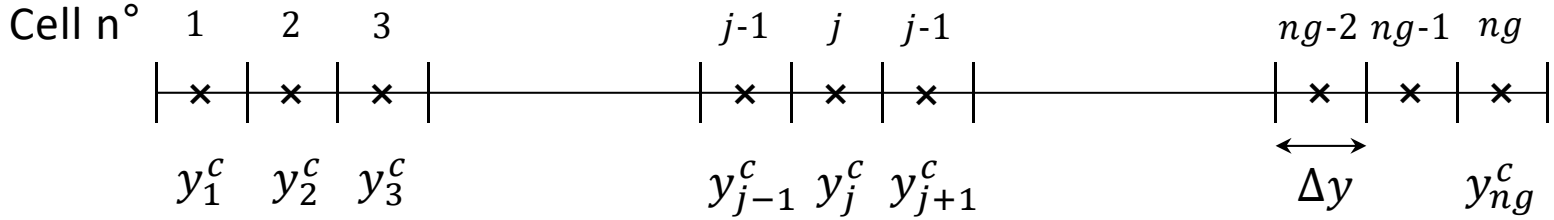
$$E_{y,sc}(y,\tau) = \int_{-\infty}^{+\infty} G_{y,\rho}(y - y')\rho_y(y')dy'$$

with $G_{y,\rho}(y) = \frac{2\lambda_e}{\varepsilon_0 \pi b^2} F(y)$, $F(y) = \mathrm{sgn}(y) \sum_n \left(\frac{J_n(\mu_n\, b/a)}{\mu_n J_n(\mu_n)}\right)^2 e^{\frac{2\pi\mu_n}{\gamma_e a}|y|}$,

$\gamma_e a = \frac{2\pi a}{\lambda_e \gamma_0}$ being the normalized drift tube radius.

Spatial discretization and particle shape

- Discretization of the klystron interaction space:

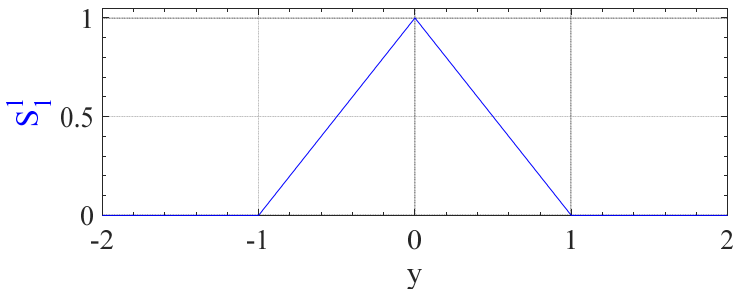


- Cell edges and centers: $y_j^e = (j-1)\Delta y$ and $y_j^c = \left(j - \frac{1}{2}\right)\Delta y$, $j = 1 : ng$
- So far, each macroparticles is considered as a point charge. To define the linear charge at any y, one replaces the Dirac distribution by integrable shape functions S so that:

$$\rho_y(y,\tau) = q_p \sum_{i=1}^{n_p} S(y - y_i(\tau)) \text{ with } \int_{-\infty}^{+\infty} S(y)dy = 1$$

- Choice of S: 1st order B-spline

$$S_{\Delta y}^1(y) = \frac{1}{\Delta y}\begin{cases} 1 - \left|\frac{y}{\Delta y}\right| & \text{for } \left|\frac{y}{\Delta y}\right| < 1 \\ 0 & \text{otherwise} \end{cases}$$



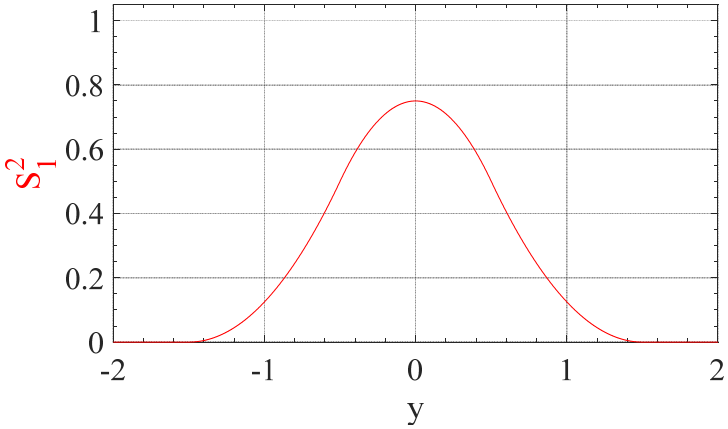
Charge projection to 1D numerical grid

- Let the particles positions be known at $y_i^n = y_i(\tau^n)$ with $\tau^n = (n-1)\Delta\tau$
- Deposition of particles charge at cell centers y_j^e and at times τ^n leads to cell-averaged charge density:

$$\rho_j^n = \frac{1}{\Delta y}\int_{y_j^e}^{y_{j+1}^e} \rho_y(y,\tau)dy = q_p \sum_{i=1}^{n_p} S_{\Delta y}^2(y_j^c - y_i^n)$$

where $S_{\Delta y}^2$ is the 2nd order B-spline:

$$S_{\Delta y}^2(y) = \frac{1}{\Delta y}\begin{cases} \frac{1}{2}\left(\frac{3}{2} - \left|\frac{y}{\Delta y}\right|\right)^2 & \text{for } \frac{1}{2} < \left|\frac{y}{\Delta y}\right| < \frac{3}{2} \\ \frac{3}{4} - \left(\frac{y}{\Delta y}\right)^2 & \text{for } \left|\frac{y}{\Delta y}\right| < \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$



with - general spline properties:

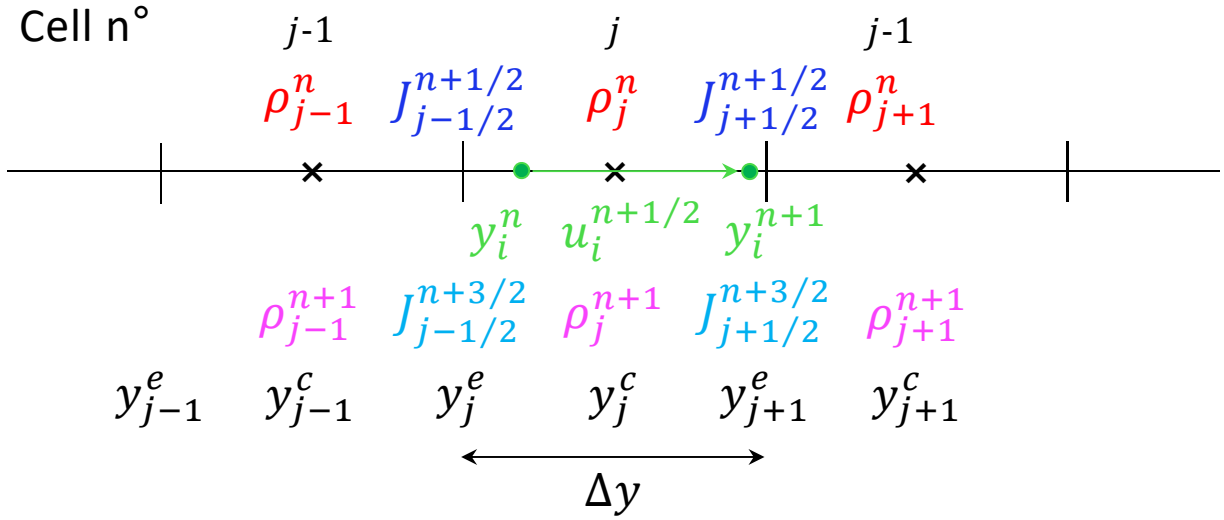
$$S_{\Delta y}^2(y_j^c - y_p) = \frac{1}{\Delta y}\int_{y_j^e}^{y_{j+1}^e} S_{\Delta y}^1(y - y_p)dy \quad \text{and} \quad \Delta y \sum_j S_{\Delta y}^2(y_j^c - y_p) = 1 \text{ for any } y_p$$

Charge conserving current deposition principle

- Choice: computation of current density at cell edges y_j^e and at times $\tau^{n+1/2}$
- Let the particles velocities be known at $u_i^{n+1/2} = u_i(\tau^{n+1/2})$
- By computing the densities of current as:

$$J_{j+1/2}^{n+1/2} = \frac{q_p}{\Delta\tau}\sum_{i=1}^{n_p} u_i^{n+1/2}\int_{\tau^n}^{\tau^{n+1}} S_{\Delta y}^1\left(y_{j+1}^e - y_i(\tau)\right)d\tau$$

the continuity equation $\frac{\partial J_y}{\partial y} + \frac{\partial \rho_y}{\partial \tau} = 0$ discretized as $\frac{J_{j+1/2}^{n+1/2} - J_{j-1/2}^{n+1/2}}{\Delta y} = -\frac{\rho_j^{n+1} - \rho_j^n}{\Delta\tau}$ is enforced

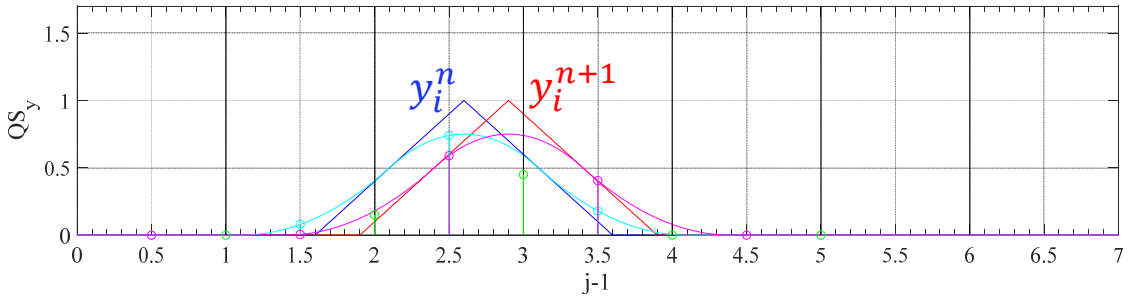


Charge conserving current deposition example

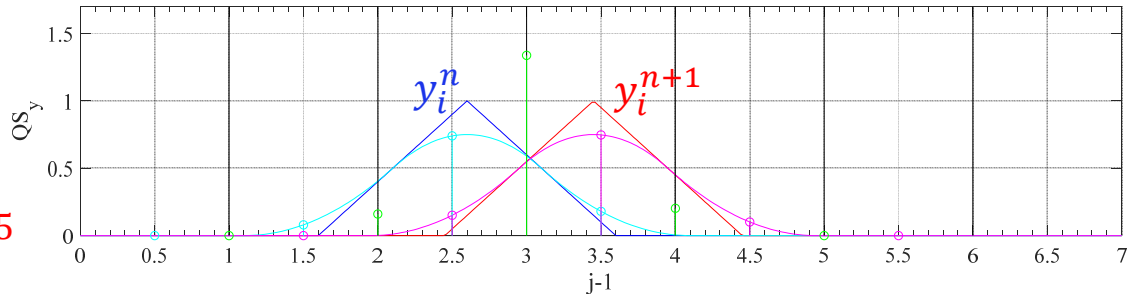
- Depending on initial position y_i^n and velocity $u_i^{n+1/2}$, there are no, 1 or 2 cell borders crossed by 1 particule during one $\Delta\tau$, each associated with different currents

$\Delta\tau = 0.025$
$\Delta y/\Delta\tau = 2$
$y_i^n = 0.13$

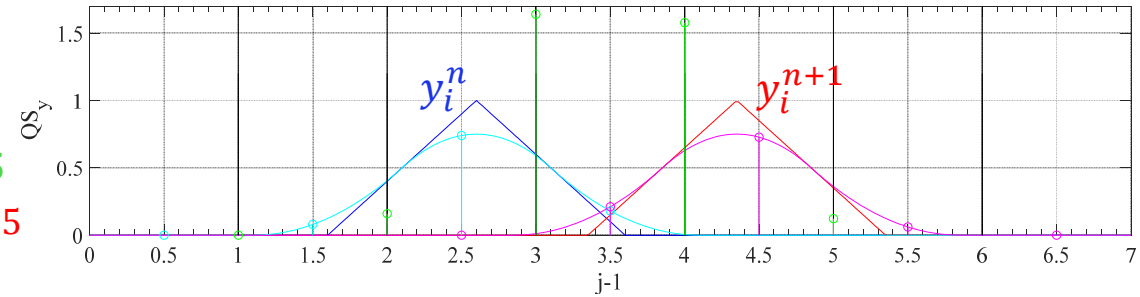
$u_i^{n+1/2} = 0.6$
$y_i^{n+1} = 0.145$



$u_i^{n+1/2} = 1.7$
$y_i^{n+1} = 0.1725$



$u_i^{n+1/2} = 3.5$
$y_i^{n+1} = 0.2175$



Grid e-fields, back-interpolation, and leap-frog

- Space-charge e-field on numerical grid at y_j^e obtained by solving convolution integral with density of charge
- RF e-fields on numerical grid at y_j^e calculated from tabulated normalized cavity fields and computation of the induced voltage v^n
- E-fields acting on each particles computed by interpolating e-fields on grid at locations of particles:

$$E_i^n = \sum_{j=1}^{ng} \frac{E_j^n + E_{j+1}^n}{2} \int_{y_j^e}^{y_{j+1}^e} S_{\Delta y}^1(y - y_i^n)dy = \sum_{j=1}^{ng} \frac{E_j^n + E_{j+1}^n}{2} \Delta y S_{\Delta y}^2(y_j^c - y_i^n)$$

- Normalized equations of motions:

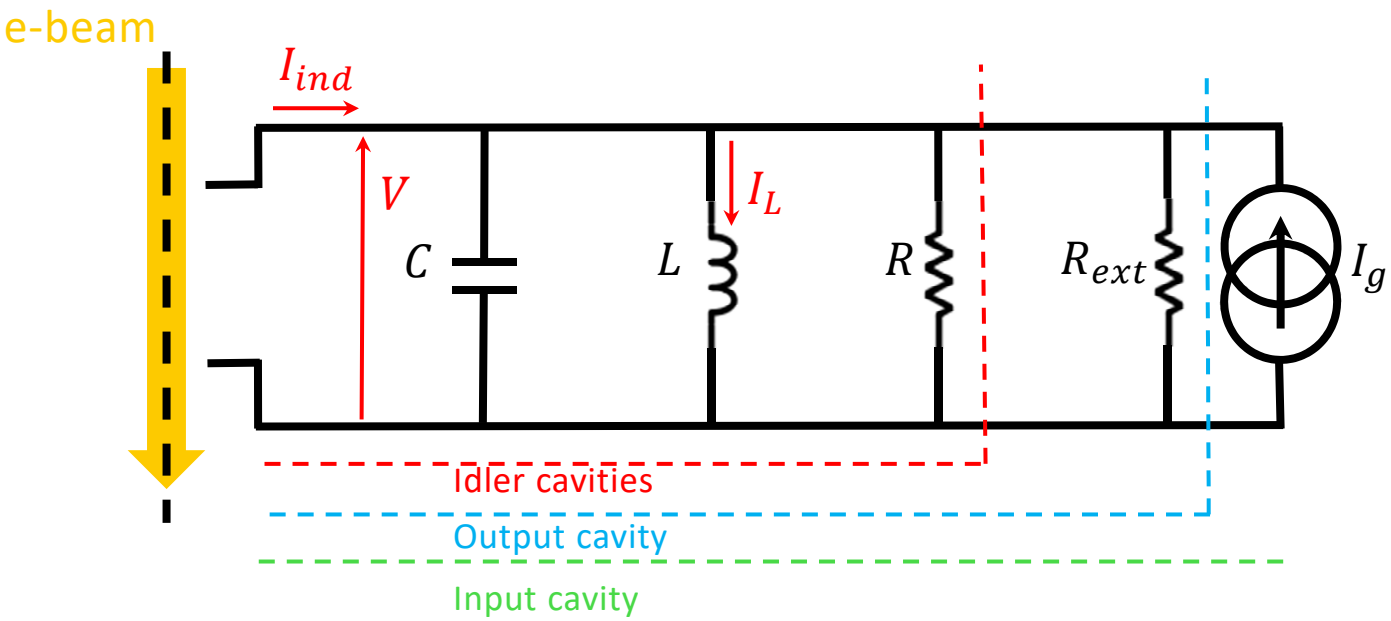
$$\frac{dy_i}{d\tau} = u_i \text{ and } \frac{d(\gamma u)_i}{d\tau} = \frac{q_p}{m_p}\frac{V_0}{v_o f \lambda_e}\left(M_r \sum_{n=1}^{N_{cav}} v_n(\tau) e_n(y_i) + \frac{E_{y,sc}(y_i(\tau))}{V_0}\right)$$

discretized in time with the classical leap-frog scheme: $y_i^{n+1} = y_i^n + u_i^{n+1/2}\Delta\tau$

$$\text{and } (\gamma u)_i^{n+3/2} = (\gamma u)_i^{n+1/2} + \frac{q_p}{m_p}\frac{V_0 \Delta\tau}{v_0 f \lambda_e}\left(M_r \sum_{n_{cav}=1}^{N_{cav}} v_{n_{cav}}^{n+1} e_{n_{cav},i}^{n+1} + \frac{E_{i,sc}^{n+1}}{V_0}\right)$$

Cavity model - General

- Klystron cavities modeled by parallel RLC circuit the current source being induced by e-beam current
- Input cavity sources: current generator and unbunched incoming e-beam (beam-loading)
- Output cavity terminated by matched load current-driven by bunched e-beam



Cavity model – System of differential equations

- Time-dependent cavity voltage V and inductance current I_L ruled by:

$$\frac{d}{dt}\begin{pmatrix} V \\ I_L \end{pmatrix} = \begin{pmatrix} -\frac{1}{RC} & -\frac{1}{C} \\ \frac{1}{L} & 0 \end{pmatrix}\begin{pmatrix} V \\ I_L \end{pmatrix} + \frac{1}{C}\begin{pmatrix} I_{ind} + I_g \\ 0 \end{pmatrix}$$ with $I_g \neq 0$ for input cavity

or, functions of cavity RF parameters, with $Q = \begin{cases} Q_l \text{ for input and output cavities} \\ Q_0 \text{ otherwise} \end{cases}$

$$\frac{d}{dt}\begin{pmatrix} V \\ I_L \end{pmatrix} = \begin{pmatrix} -\frac{\omega_0}{Q} & -\omega_0(R/Q) \\ \frac{\omega_0}{R/Q} & 0 \end{pmatrix}\begin{pmatrix} V \\ I_L \end{pmatrix} + \omega_0(R/Q)\begin{pmatrix} I_{ind} + I_g \\ 0 \end{pmatrix}$$

- With normalized cavity voltage v and currents normalized to I_0:

$$\frac{1}{2\pi}\frac{d}{d\tau}\begin{pmatrix} v \\ i_L \end{pmatrix} = \begin{pmatrix} -a_c & -c_c \\ \frac{b_c}{c_c} & 0 \end{pmatrix}\begin{pmatrix} v \\ i_L \end{pmatrix} + c_c\begin{pmatrix} i_{ind} + i_g \\ 0 \end{pmatrix}$$

with:

$a_c = \frac{\omega_0}{\omega Q}$, $b_c = \left(\frac{\omega_0}{\omega}\right)^2$ and $c_c = G_0(R/Q)\left(\frac{\omega_0}{\omega}\right)$, G_0 being the static beam admittance

Convergence acceleration

- To accelerate the convergence to steady state, change the transient behavior of the above system. Set replacement system:

$$\frac{1}{2\pi}\frac{d}{d\tau}\begin{pmatrix} v \\ i_L \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} v \\ i_L \end{pmatrix} + \begin{pmatrix} B_1(i_{ind} + i_g) \\ B_2(i_{ind} + i_g) \end{pmatrix}$$

Steady-state of initial system given by: $\frac{v}{i_{ind} + i_g} = z_c$ and $\frac{i_L}{i_{ind} + i_g} = -j\frac{b_c z_c}{c_c}$

- Choosing $det(A)$ and $tr(A)$ - or the eigenvalues of A - and defining the complex quantity:

$$\Delta_A = \begin{vmatrix} j - A_{11} & A_{12} \\ A_{21} & j - A_{22} \end{vmatrix} = det(A) - 1 - jtr(A)$$

the constraints on A's and B's for the steady-state of the replacement system to be identical to the original one are:

$$\frac{1}{\Delta_A}\begin{pmatrix} j - A_{22} & A_{12} \\ A_{21} & j - A_{11} \end{pmatrix}\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \begin{pmatrix} \frac{v}{i_{ind} + i_g} \\ \frac{i_L}{i_{ind} + i_g} \end{pmatrix} \quad \text{and} \quad \begin{cases} A_{11} + A_{22} = tr(A) \\ A_{11}A_{22} - A_{12}A_{21} = det(A) \end{cases}$$

Final replacement system and leap-frog

- The above system is solved to obtain real A_{ij} and B_i

- For each cavity, voltage v and current i_L solved with the leap-frog scheme:

$$\frac{v^{n+1}-v^n}{2\pi\Delta\tau} = \frac{A_{11}}{2}\left(v^{n+1}+v^n\right) + \frac{A_{21}}{2} i_L^{n+1/2} + B_1\left(i_{ind}^{n+1/2} + i_g^{n+1/2}\right)$$

$$\frac{i_L^{n+3/2}-i_L^{n+1/2}}{2\pi\Delta\tau} = A_{21}v^n + \frac{A_{22}}{2}\left(i_L^{n+3/2}+i_L^{n+1/2}\right) + \frac{B_2}{2}\left(i_{ind}^{n+3/2}+i_g^{n+3/2}+i_{ind}^{n+1/2}+i_g^{n+1/2}\right)$$

- Induced current in cavity defined as:

$$i_{ind,n_{cav}}^{n+1/2} = F_{coef,harm}\left(M_r \sum_{j=1}^{ng} \Delta y \left(J_{j-1/2}^{n+1/2} - J_{j0}\right) e_{n_{cav},j-1/2}\right)$$

with $e_{j-1/2}$ normalized cavity e-field at y_j^e

- Current generator normalized to the beam current i_g chosen as a sin time-domain variation and an amplitude function of input power

SLAC 5045 S-band klystron input data

(*)

Operating frequency (MHz)	Beam voltage (kV)	Beam current (A)	Beam radius (cm)	Drift radius (cm)
2856	320	362	1.10	1.59

(*)

Cavity No.	Cavity frequency (MHz)	$R/Q^{(**)}$ (Ω)	Q_0	Q_{ext}	Gap length (mm)	$M_l^{(**)}$	Drift length (cm)
1	2860	58.2	2000	175	6.76	0.726	-
2	2855	75.1	2000	-	7.19	0.725	5.55
3	2877	68.3	2000	-	8.36	0.717	5.55
4	2887	79.6	2000	-	11.18	0.703	5.55
5	2935	89.4	2000	-	12.01	0.690	28.53
6	2852	96.9	2000	16.5	16.59	0.648	10.36

(*) from A. Jensen with AJDISK, priv.com. Jan. 2012 (**) at radius $0.707b$

```
% Data for SLAC 5045 klystron - Ncav=6
% tstart ncyclmax nt_per_cycl dyovdt ystart yend np_per_cell flrf spch Ncav_op  Pin
  0      35        80          2      -2     8    40          1    0    6        1e3
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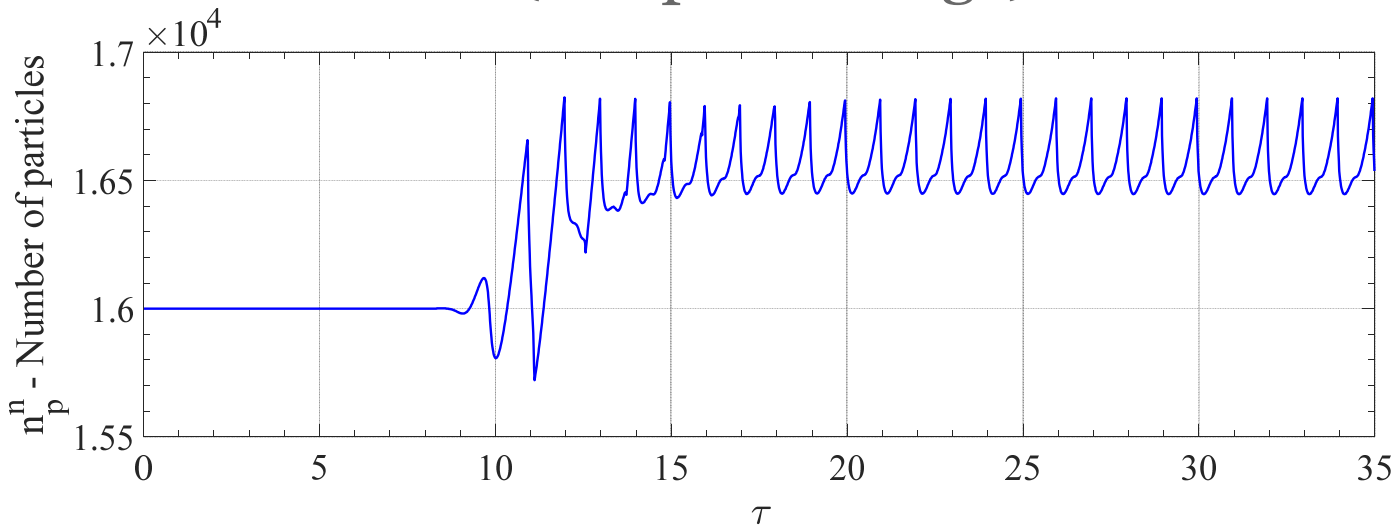
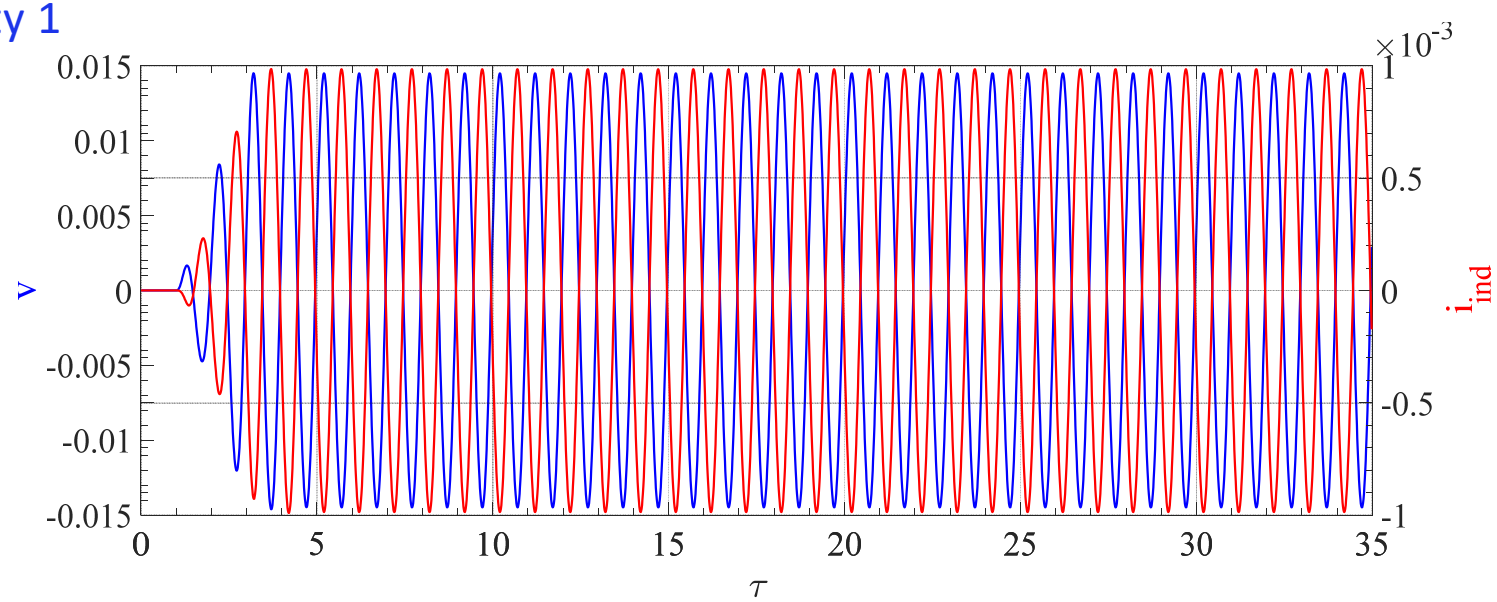
SLAC 5045 klystron numerical experiment (no space charge)



Cavity 1



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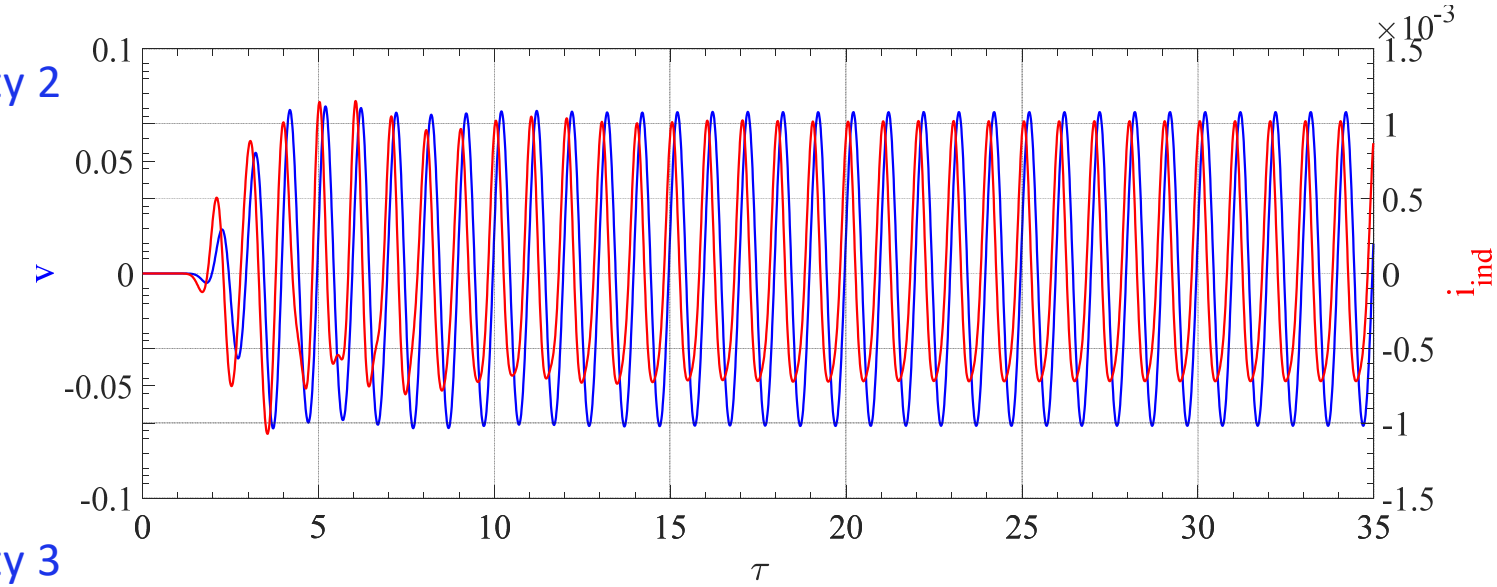
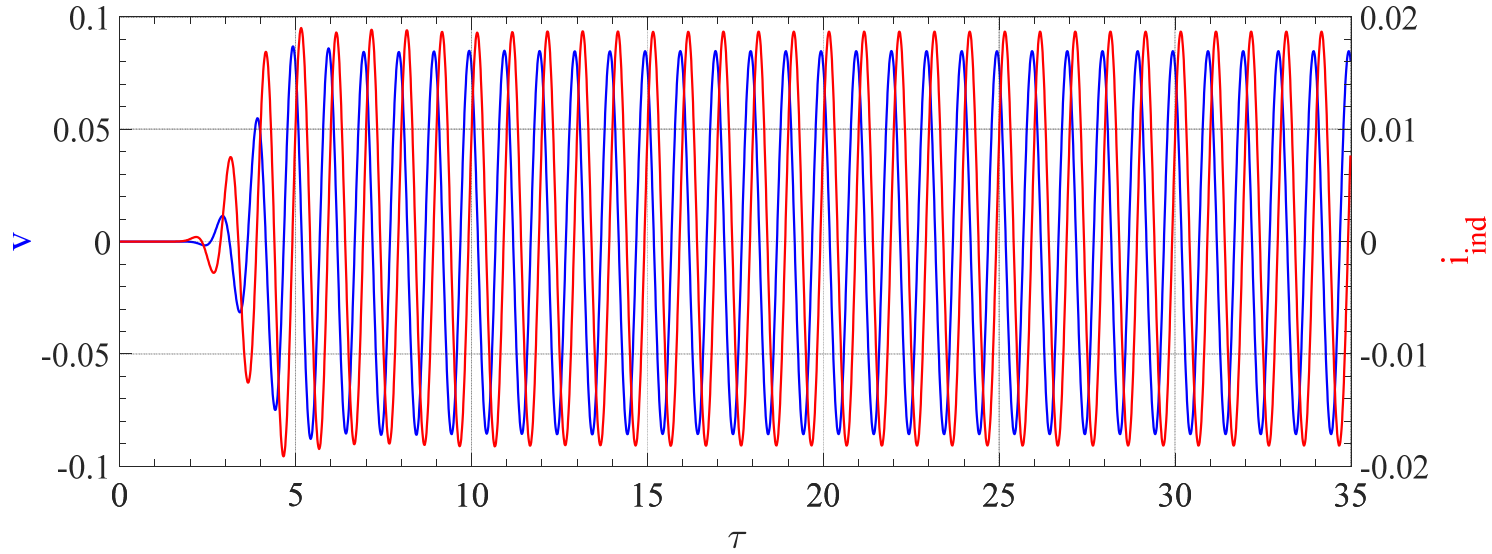
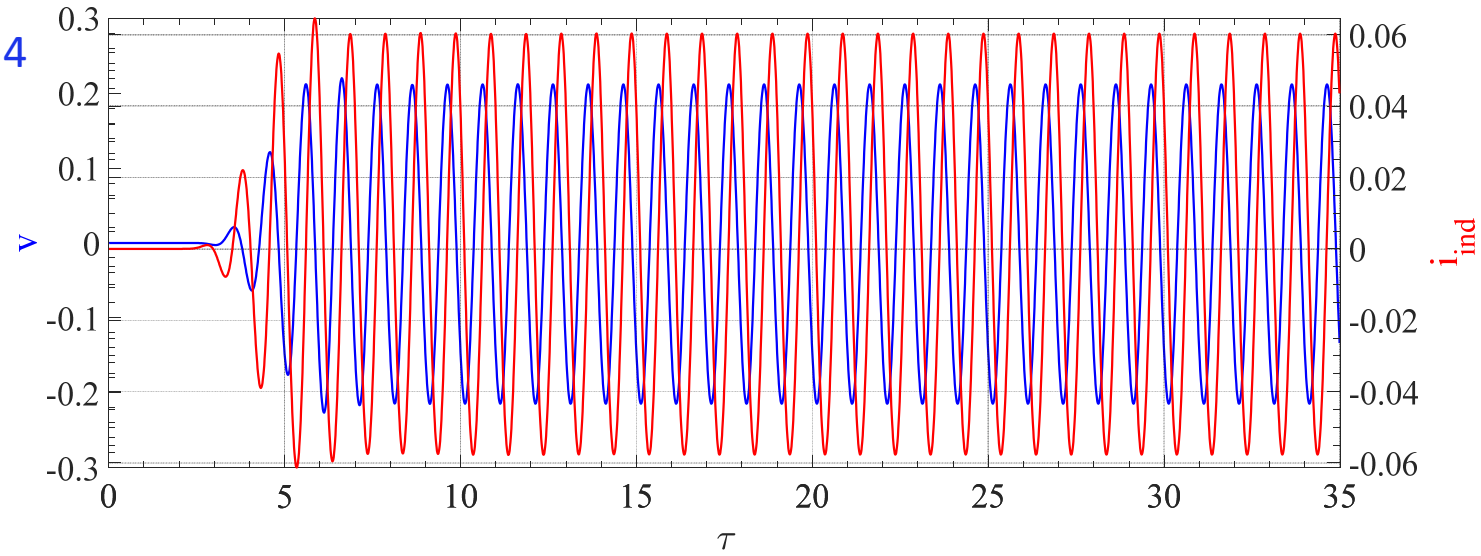
Cavity 2



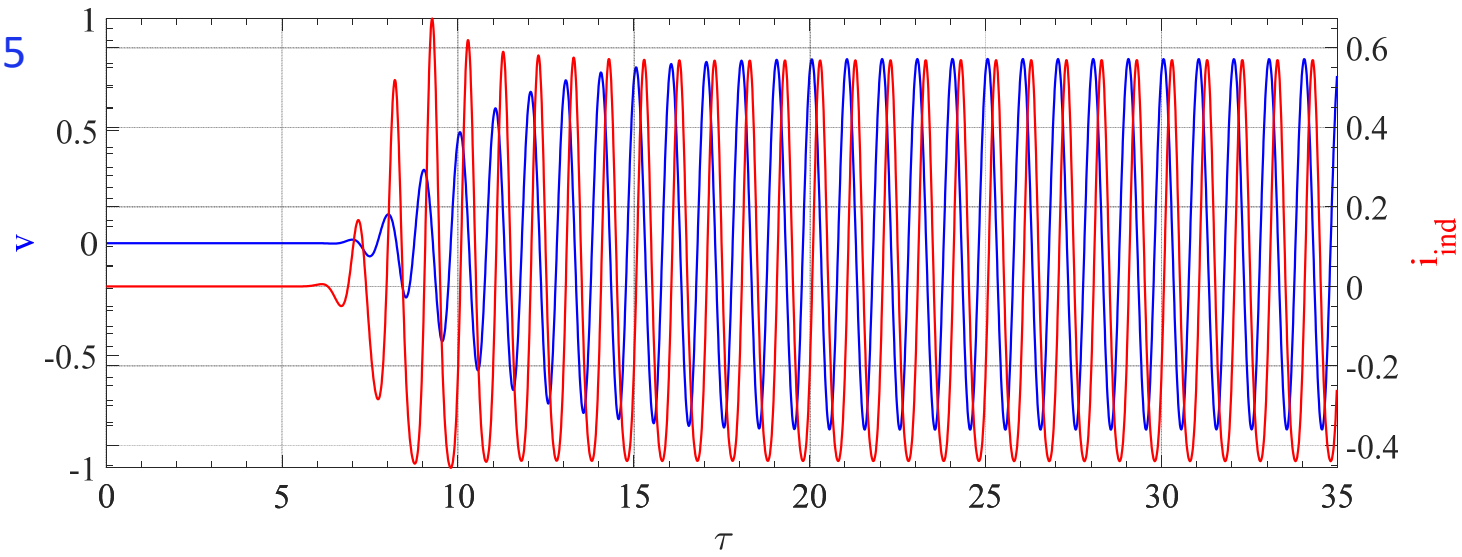
Cavity 3



Cavity 4



Cavity 5



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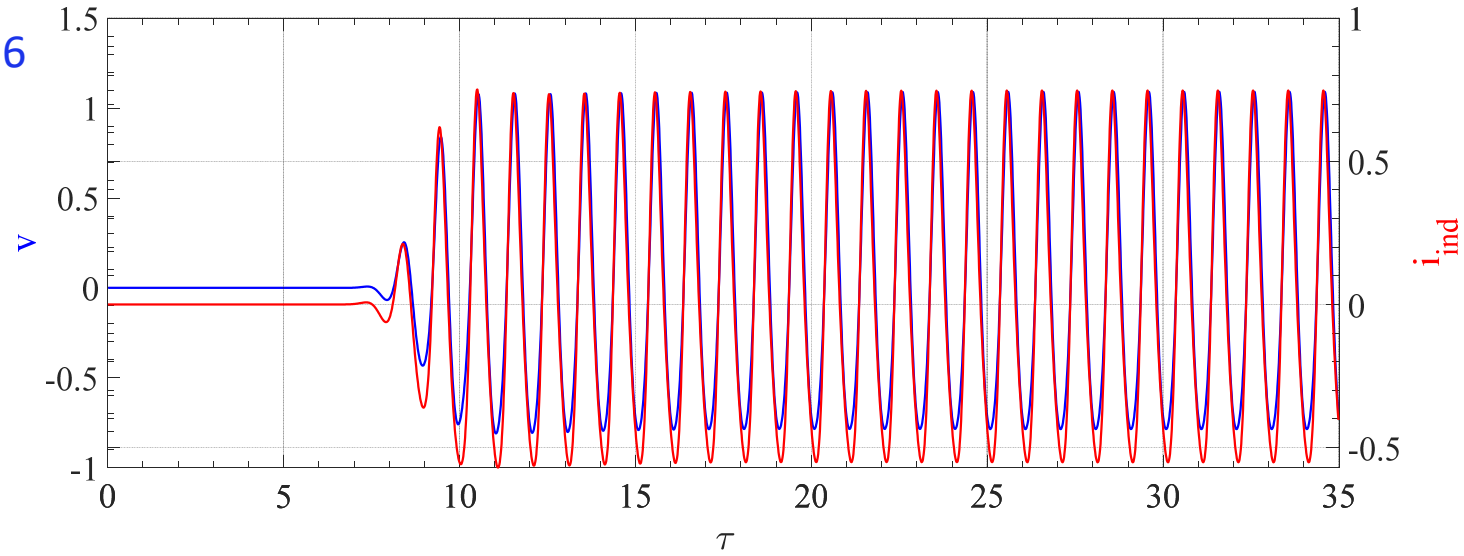
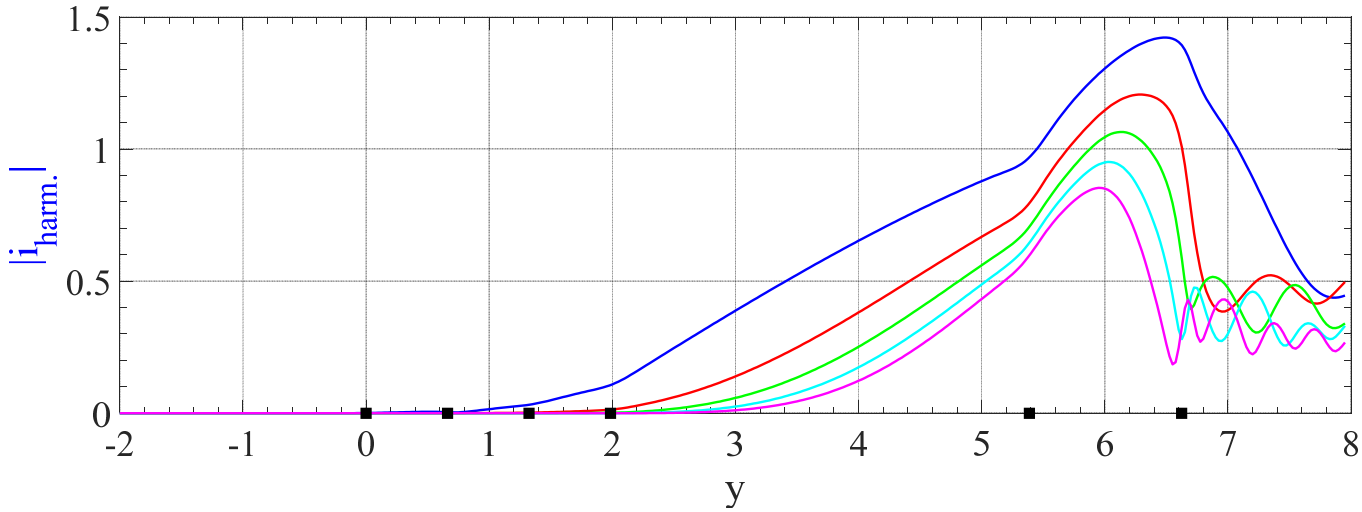
Cavity 6



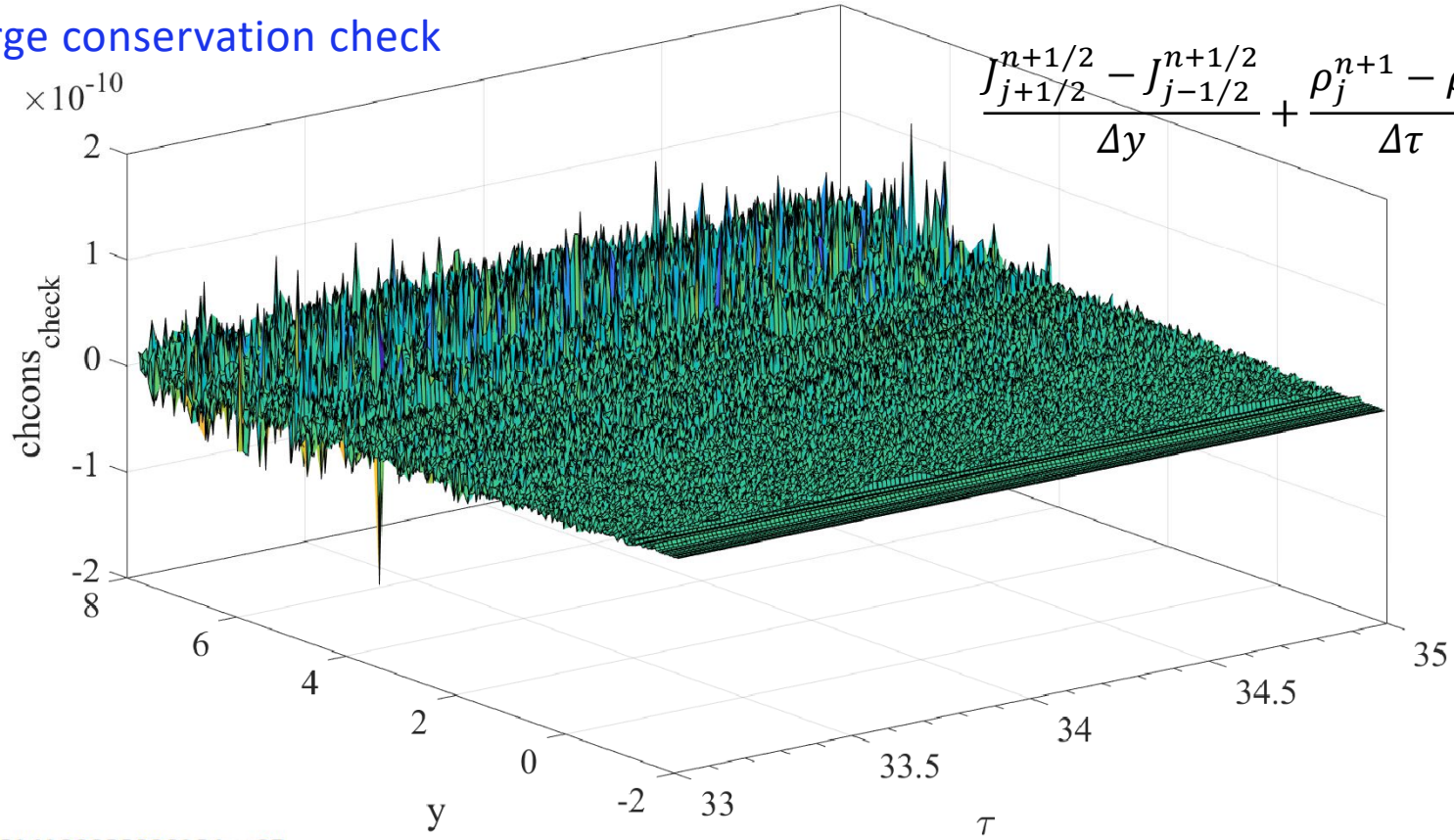
Beam current harmonics



SLAC 5045 klystron numerical experiment

Charge conservation check

$$\frac{J_{j+1/2}^{n+1/2} - J_{j-1/2}^{n+1/2}}{\Delta y} + \frac{\rho_j^{n+1} - \rho_j^n}{\Delta \tau}$$




```
Pout =

     3.514120055223154e+07


GdB =

  45.458165945042659

Elapsed time is 206.631147 seconds.
```

References - Numerical methods

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