Space charge: Theories and comparison of ELEGANT, GPT and SAD

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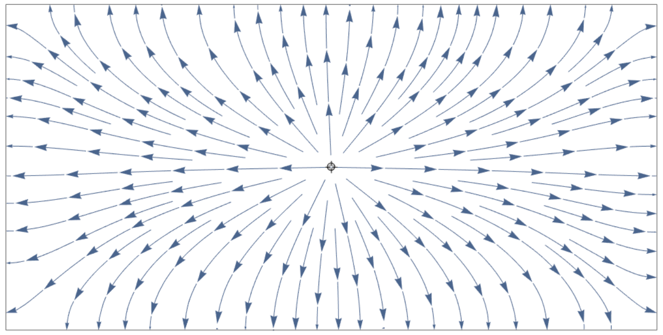
cERL-FEL meeting, Oct. 22, 2020

Outline

- ➢ **Impedance theory of space charge**
- ➢ **Models for LSC and TSC in ELEGANT, GPT and SAD**
- ➢ **Summary and outlook**

1. Impedance theory of SC



Fundamental definitions

Consider a charged particle moving in parallel to the axis of a rectangular waveguide with its transverse dimensions given by $-a/2 < x < a/2$ and $-b/2 < y < b/2$. The waveguide has infinite length in the z direction with its walls assumed to be perfectly conductive, and the particle has constant velocity $\vec{v} = \vec{i}_z v$. With the charge density defined by Dirac delta functions as

$$\varrho(\vec{r}, t) = q_0 \delta(x - x_0)\delta(y - y_0)\delta(z - vt), \tag{1}$$

the current density is given by $\vec{\mathcal{J}}(\vec{r}, t) = \varrho(\vec{r}, t)\vec{v}$. One can apply them to the Maxwell's equations with boundary conditions and obtain the time-varying electromagnetic fields $\vec{\mathcal{E}}(\vec{r}, t)$ and $\vec{\mathcal{B}}(\vec{r}, t)$.

According to the standard impedance theory [A. Chao, 1993], a test charged particle q_1 with coordinates $\vec{r}_1 = (x_1, y_1, s_1)$ follows q_0 with the same velocity but at a time delay of $\tau = z/v$, e.g. $s_1 = v(t - \tau)$. The Lorentz force acted on q_1 is then given by

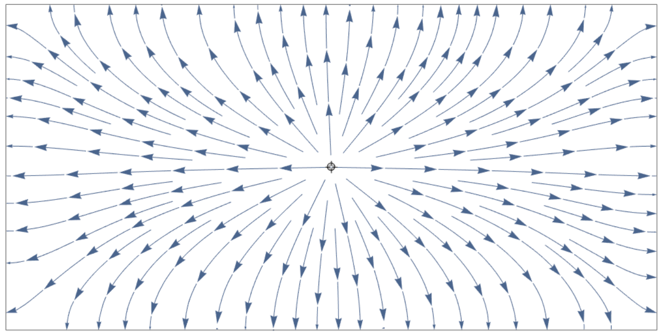
$$\vec{\mathcal{F}}(\vec{r}_1, \vec{r}_0; t) = q_1 \left[\vec{\mathcal{E}}(\vec{r}_1, \vec{r}_0; t) + \vec{v} \times \vec{\mathcal{B}}(\vec{r}_1, \vec{r}_0; t)\right]. \tag{2}$$

The impulse kick applied to q_1 when it travels by a length of L is calculated by integrating the Lorentz force as

$$\overline{\vec{\mathcal{F}}}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) = \int_{\tau}^{\tau + \frac{L}{v}} dt\ v\vec{\mathcal{F}}(\vec{r}_1, \vec{r}_0; t). \tag{3}$$

The subscripts $\perp$ in Eq. (3) represent the transverse coordinates, i.e. $\vec{r}_{1\perp} = (x_1, y_1)$ and $\vec{r}_{0\perp} = (x_0, y_0)$. The quantity $\overline{\vec{\mathcal{F}}}$ is called the wake potential, which is a function of τ and the

1. Impedance theory of SC



Fundamental definitions

transverse coordinates of source and test particles. Then the longitudinal and transverse wake functions $W_{\parallel}(\vec{r}_{2\perp}, \vec{r}_{1\perp}; \tau)$ and $\vec{W}_{\perp}(\vec{r}_{2\perp}, \vec{r}_{1\perp}; \tau)$ are defined as follows

$$W_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) = -\frac{1}{q_0 q_1}\overline{\mathcal{F}}_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau), \quad (4a)$$

$$\vec{W}_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) = \frac{1}{q_0 q_1}\overline{\vec{\mathcal{F}}}_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau). \quad (4b)$$

Using Fourier transform, one can calculate the spectrum of the wake functions, so called impedance, as

$$Z_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \omega) = \int_{-\infty}^{\infty} d\tau \; W_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) e^{i\omega\tau}, \quad (5a)$$

$$\vec{Z}_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \omega) = \kappa \int_{-\infty}^{\infty} d\tau \; \vec{W}_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) e^{i\omega\tau}, \quad (5b)$$

with $\kappa = \frac{i}{v/c}$ [K.Y. Ng, 2006]. Then the wake functions expressed by inverting the above Fourier transforms are

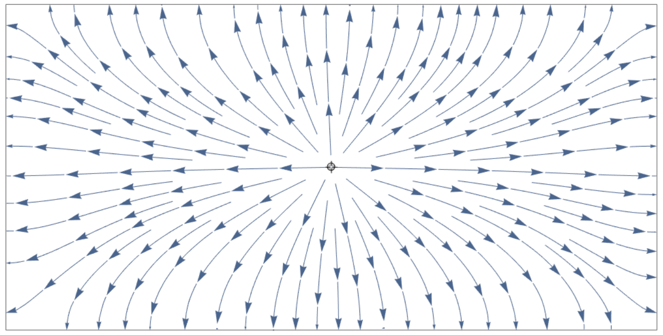
$$W_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \; Z_{\parallel}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \omega) e^{-i\omega\tau}, \quad (6a)$$

$$W_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \tau) = \frac{1}{2\pi\kappa} \int_{-\infty}^{\infty} d\omega \; Z_{\perp}(\vec{r}_{1\perp}, \vec{r}_{0\perp}; \omega) e^{-i\omega\tau}. \quad (6b)$$

The imaginary constant i appears in Eqs. (5b) and (6b) due to a historical convention. The main task is then to find the explicit forms of Eqs. (5a) and (5b) in terms of eigenmodes of the rectangular waveguide.

1. Impedance theory of SC

Mode expansion method



For a passive waveguide, the delta function of z in Eq. (1) can be replaced by its Fourier transform as

$$\delta(z - vt) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ik(z-vt)}\, dk. \tag{7}$$

The delta function of transverse coordinates can be expanded into the summation of the eigenmodes of the rectangular waveguide as follows

$$\delta(\vec{r}_\perp - \vec{r}_{0\perp}) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \phi_{mn\nu}(\vec{r}_\perp)\, \phi_{mn\nu}(\vec{r}_{0\perp}), \tag{8}$$

where $\nu = x,\ y$, or z, and the subscript $\perp$ denotes the transverse coordinates. And the complete set of orthonormal eigenfunction for the x, y and z directions are

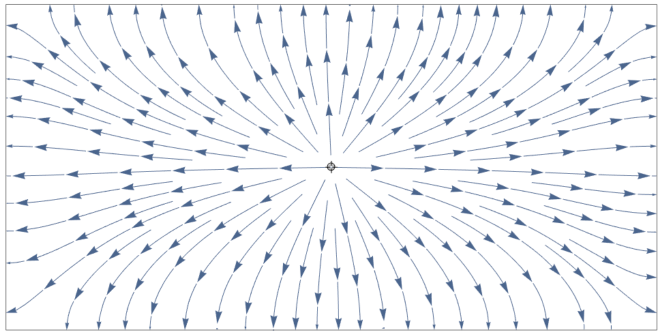
$$\phi_{mnx}(\vec{r}_\perp) = \frac{2}{\sqrt{(1+\delta_{m0})\, ab}} C_x(x) S_y(y), \tag{9a}$$

$$\phi_{mny}(\vec{r}_\perp) = \frac{2}{\sqrt{(1+\delta_{n0})\, ab}} S_x(x) C_y(y), \tag{9b}$$

$$\phi_{mnz}(\vec{r}_\perp) = \frac{2}{\sqrt{ab}} S_x(x) S_y(y), \tag{9c}$$

where δ_{m0} and δ_{n0} are Kronecker deltas. Here we define $C_x(x) \equiv \cos(k_x(x + a/2))$, $S_x(x) \equiv \sin(k_x(x + a/2))$, $C_y(y) \equiv \cos(k_y(y + b/2))$, and $S_y(y) \equiv \sin(k_y(y + b/2))$ with the transverse wave numbers $k_x = m\pi/a$ and $k_y = n\pi/b$.

1. Impedance theory of SC



Mode expansion method

Here we omit the detailed calculations and directly give the explicit formulations of the vector potential:

$$\vec{A}\left(\vec{r},k\right) = \mu_0 q_0 \beta^2 \gamma^2 \vec{i}_z \sum_{m,n\geq 0} \frac{\phi_{mnz}\left(\vec{r}_\perp\right)\phi_{mnz}\left(\vec{r}_{0\perp}\right)}{k^2+\beta^2\gamma^2(k_x^2+k_y^2)} e^{ikz/\beta}, \tag{13}$$

with the relative velocity $\beta = v/c$ and Lorentz factor γ. The above vector potential can be applied to calculate the electromagnetic fields and then the space-charge induced impedance. Again with the detailed calculations omitted, we directly give the explicit form of impedance per unit length:

$$\frac{Z_\parallel(k)}{L} = \frac{4i\mu_0 kc}{ab} \sum_{m,n\geq 0} \frac{\phi'_{mnz}\left(\vec{r}_{1\perp}\right)\phi'_{mnz}\left(\vec{r}_{0\perp}\right)}{k^2+\beta^2\gamma^2(k_x^2+k_y^2)}, \tag{14a}$$

$$\frac{Z_x(k)}{L} = \frac{-4\mu_0 \beta c\kappa}{ab} \sum_{m,n\geq 0} \frac{k_x\phi'_{mnx}\left(\vec{r}_{1\perp}\right)\phi'_{mnz}\left(\vec{r}_{0\perp}\right)}{k^2+\beta^2\gamma^2(k_x^2+k_y^2)}, \tag{14b}$$

$$\frac{Z_y(k)}{L} = \frac{-4\mu_0 \beta c\kappa}{ab} \sum_{m,n\geq 0} \frac{k_y\phi'_{mny}\left(\vec{r}_{1\perp}\right)\phi'_{mnz}\left(\vec{r}_{0\perp}\right)}{k^2+\beta^2\gamma^2(k_x^2+k_y^2)}, \tag{14c}$$

$$Z_x(k) = \frac{-i\beta\kappa}{k}\frac{\partial Z_\parallel(k)}{\partial x_1}$$

$$Z_y(k) = \frac{-i\beta\kappa}{k}\frac{\partial Z_\parallel(k)}{\partial y_1}$$

where the unnormalized eigenfunctions are defined as

$$\phi'_{mnx}\left(x,y\right) = C_x(x)S_y(y), \tag{15a}$$

$$\phi'_{mny}\left(x,y\right) = S_x(x)C_y(y), \tag{15b}$$

$$\phi'_{mnz}\left(x,y\right) = S_x(x)S_y(y). \tag{15c}$$

1. Impedance theory of SC

Free-space SC impedance with transverse bi-Gaussian distribution

Consider the case of free space and transverse bi-gaussian beam distribution, we can find

$$\frac{Z_{\parallel}(k)}{L} = \frac{i\mu_0 kc}{4\pi\beta^2\gamma^2}\int_0^\infty dt' \frac{1}{(t'+2\sigma_x^2)^{1/2}(t'+2\sigma_y^2)^{1/2}} e^{-\frac{(x-x_c)^2}{t'+2\sigma_x^2}-\frac{(y-y_c)^2}{t'+2\sigma_y^2}} e^{-\frac{k^2 t'}{4\beta^2\gamma^2}}, \tag{21a}$$

$$\frac{Z_x(k)}{L} = -\frac{\mu_0 c\kappa}{2\pi\beta\gamma^2}\int_0^\infty dt' \frac{x-x_c}{(t'+2\sigma_x^2)^{3/2}(t'+2\sigma_y^2)^{1/2}} e^{-\frac{(x-x_c)^2}{t'+2\sigma_x^2}-\frac{(y-y_c)^2}{t'+2\sigma_y^2}} e^{-\frac{k^2 t'}{4\beta^2\gamma^2}}, \tag{21b}$$

$$\frac{Z_y(k)}{L} = -\frac{\mu_0 c\kappa}{2\pi\beta\gamma^2}\int_0^\infty dt' \frac{y-y_c}{(t'+2\sigma_x^2)^{1/2}(t'+2\sigma_y^2)^{3/2}} e^{-\frac{(x-x_c)^2}{t'+2\sigma_x^2}-\frac{(y-y_c)^2}{t'+2\sigma_y^2}} e^{-\frac{k^2 t'}{4\beta^2\gamma^2}}. \tag{21c}$$

3D LSC and TSC model

We can rewrite the above equations as follows:

$$\frac{Z_{\parallel}(k)}{L} = \frac{i\mu_0 c}{4\pi\beta^2\gamma^2} F_z(x,y,r,k), \tag{22a}$$

$$\frac{Z_x(k)}{L} = -\frac{\mu_0 c\kappa(x-x_c)}{4\pi\beta\gamma^2\sigma_x^2} F_x(x,y,r,k), \tag{22b}$$

$$\frac{Z_y(k)}{L} = -\frac{\mu_0 c\kappa(y-y_c)}{4\pi\beta\gamma^2\sigma_x^2} F_y(x,y,r,k), \tag{22c}$$

with

$$F_z(x,y,r,k) = k\int_0^\infty dt \frac{1}{(t+1)^{1/2}(t+r^2)^{1/2}} e^{-\frac{(x-x_c)^2}{2\sigma_x^2(t+1)}-\frac{(y-y_c)^2}{2\sigma_x^2(t+r^2)}} e^{-\frac{k^2\sigma_x^2 t}{2\beta^2\gamma^2}}, \tag{23a}$$

$$F_x(x,y,r,k) = \int_0^\infty dt \frac{1}{(t+1)^{3/2}(t+r^2)^{1/2}} e^{-\frac{(x-x_c)^2}{2\sigma_x^2(t+1)}-\frac{(y-y_c)^2}{2\sigma_x^2(t+r^2)}} e^{-\frac{k^2\sigma_x^2 t}{2\beta^2\gamma^2}}, \tag{23b}$$

$$F_y(x,y,r,k) = \int_0^\infty dt \frac{1}{(t+1)^{1/2}(t+r^2)^{3/2}} e^{-\frac{(x-x_c)^2}{2\sigma_x^2(t+1)}-\frac{(y-y_c)^2}{2\sigma_x^2(t+r^2)}} e^{-\frac{k^2\sigma_x^2 t}{2\beta^2\gamma^2}}. \tag{23c}$$

Longitudinal damping term

Transverse damping term

Here we define $r = \sigma_y/\sigma_x$.

1. Impedance theory of SC

Free-space SC impedance with transverse bi-Gaussian distribution

The convergence property of $F_z(x,y,r,k)$ very depends on k, therefore in Eq. (22a) we merge k into F_z. The exponential term in Eqs. (23) plays a role of damping and sets a threshold of the frequency:

$$k_{th} = \frac{\sqrt{2}\beta\gamma}{\min[\sigma_x,\sigma_y]}. \tag{24}$$

With $k \gg k_{th}$, the space charge impedance is strongly suppressed, so that high frequency impedance can be neglected. For a Gaussian bunch with length σ_z, the typical frequency is $k \sim 1/\sigma_z$. If $1/\sigma_z \ll k_{th}$ is satisfied, the damping term in Eqs. (23b) and (23c) can be ignored and the transverse space charge impedance can be approximated with

$$F_x(x,y,r,k) = \int_0^\infty dt \frac{1}{(t+1)^{3/2}(t+r^2)^{1/2}} e^{-\frac{(x-x_c)^2}{2\sigma_x^2(t+1)} - \frac{(y-y_c)^2}{2\sigma_x^2(t+r^2)}}, \tag{25a}$$

$$F_y(x,y,r,k) = \int_0^\infty dt \frac{1}{(t+1)^{1/2}(t+r^2)^{3/2}} e^{-\frac{(x-x_c)^2}{2\sigma_x^2(t+1)} - \frac{(y-y_c)^2}{2\sigma_x^2(t+r^2)}}. \tag{25b}$$

In the presence of microstructures with dimension of Δz, σ_z should be replaced by Δz correspondingly.

Condition of neglecting high-frequency SC impedance

1. Impedance theory of SC

Free-space SC impedance with transverse bi-Gaussian distribution

The longitudinal impedance expressed by Eq. (23a) is not integrable except the special case of $r = 1$ and $\sigma_x = \sigma_y = \sigma$:

$$F_z(0,0,1,k) = k e^{\frac{k^2\sigma^2}{2\beta^2\gamma^2}} \Gamma\left(\frac{k^2\sigma^2}{2\beta^2\gamma^2}\right), \tag{27}$$

where the incomplete Gamma function $\Gamma(x)$ is defined as

$$\Gamma(x) = \int_x^\infty \frac{e^{-t}}{t} dt. \tag{28}$$

When $k \ll \sqrt{2}\beta\gamma/\sigma$, the asymptotic expression is

$$F_z(0,0,1,k) \approx -k\left(\ln\frac{k^2\sigma^2}{2\beta^2\gamma^2} + \gamma_E\right), \tag{29}$$

with $\gamma_E \approx 0.577216$ the Euler's constant. For the case of unequal horizontal and vertical beam sizes, a good approximation is

$$F_z(0,0,r,k) \approx -k\left(\ln\frac{k^2\sigma_x^2(1+r^2)}{4\beta^2\gamma^2} + \gamma_E\right), \tag{30}$$

Simple model 1

In Ref. [M. Venturini, PRST-AB 11, 034401 (2008)] it was proposed to use

$$F_V(k) \approx -k\left(\ln\frac{k^2 r_b^2}{4\beta^2\gamma^2} + 2\gamma_E - 1\right), \tag{31}$$

Simple model 2

with $r_b \approx 1.747(\sigma_x + \sigma_y)/2$. In the ELEGANT code, the 1D model is expressed by a scaling factor of

$$F_E(k) = \frac{4k}{\xi_\sigma^2}\left[1 - \xi_\sigma K_1(\xi_\sigma)\right], \tag{32}$$

Simple model 3

where $\xi_\sigma = kr_b/(\beta\gamma)$ and $K_1(x)$ is the modified Bessel function of the second kind. Note that originally the above equation was derived with the assumption of transversely uniform beam density, and we also recovered the velocity β since our theory is valid for arbitrary beam energy.

1. Impedance theory of SC

1D LSC impedance model (ELEGANT):

$$\frac{Z_{\mathrm{LSC}}(k)}{L} = \frac{iZ_0}{\pi k r_b^2}\left[1 - \frac{kr_b}{\gamma}K_1\left(\frac{kr_b}{\gamma}\right)\right] \qquad r_b = 1.747(\sigma_x + \sigma_y)/2$$

Z. Huang et al., Phys. Rev. ST Accel. Beams 7 074401 (2004)
M. Venturini, Phys. Rev. ST Accel. Beams 11 034401 (2008)

3D TSC impedance model (Derived from Eqs.(25), SAD and ELEGANT):

$$\frac{W_{\mathrm{x}}(x,y,z) - iW_{\mathrm{y}}(x,y,z)}{L} = \frac{-iZ_0 c}{2\pi\gamma^2}\psi(z)\frac{\sqrt{\pi}}{2(\sigma_x^2-\sigma_y^2)}\left[w(a+ib) - e^{-B}w(ar + i\frac{b}{r})\right]$$

$$a = \frac{x}{\sqrt{2(\sigma_x^2-\sigma_y^2)}} \qquad b = \frac{y}{\sqrt{2(\sigma_x^2-\sigma_y^2)}} \qquad r = \frac{\sigma_y}{\sigma_x}$$

$$B = a^2(1-r^2) + b^2(\frac{1}{r^2}-1) = \frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2}$$

Application conditions: Assume σx and σy are z-independent inside the bunch, and:

$$\gamma\sigma_z \gg \sigma_\perp$$
$$\sigma_\perp = \mathrm{Min}[\sigma_x, \sigma_y]$$

ψ(z): Longitudinal density is good enough, no need to use Gaussian distribution.
For Gaussian distribution (Used in ELEGANT and SAD):

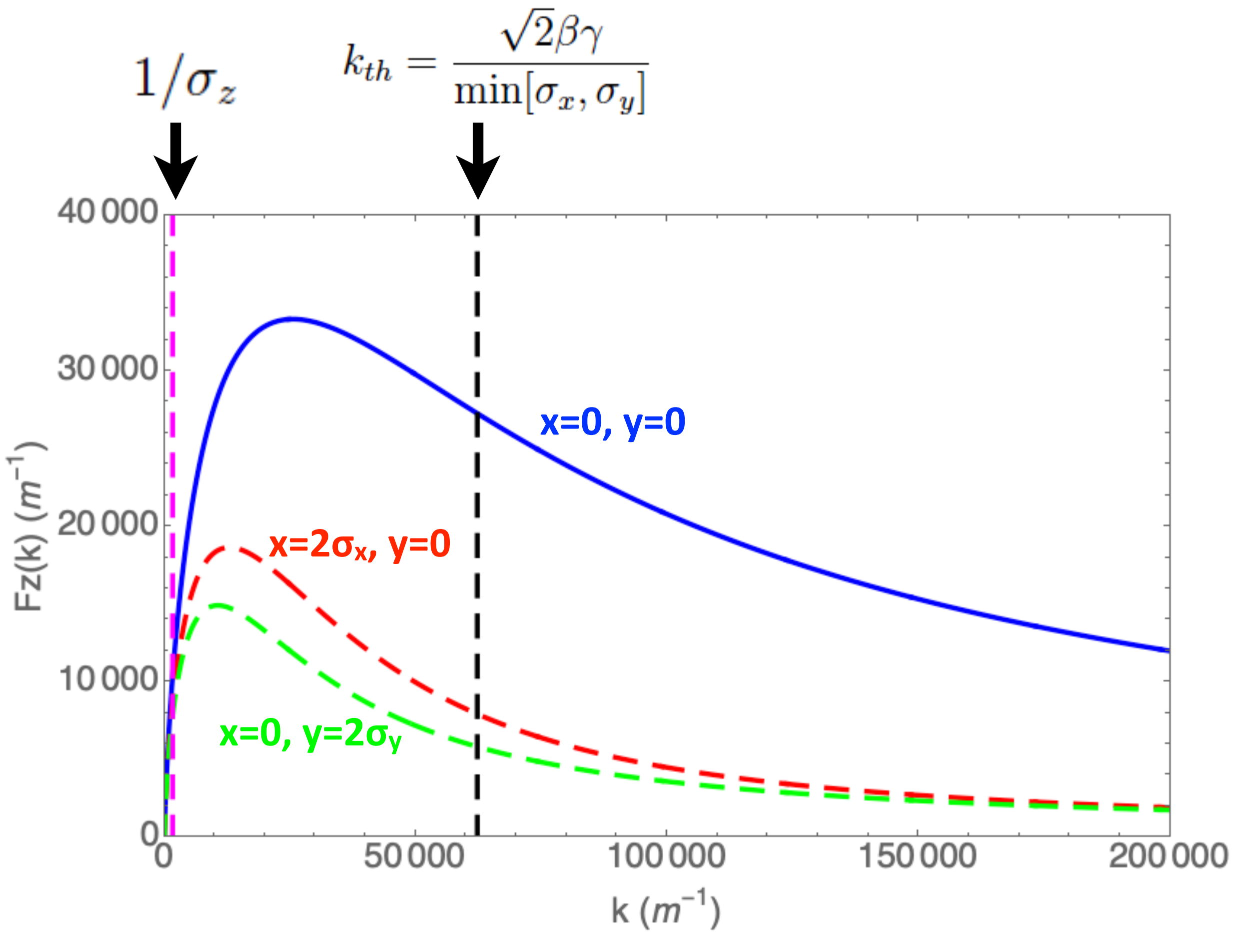
$$\psi(z) = \frac{1}{\sqrt{2\pi}\sigma_z}e^{-\frac{z^2}{2\sigma_z^2}}$$

A. Xiao et al., PAC'07, also FERMILAB-CONF-07-702-AD

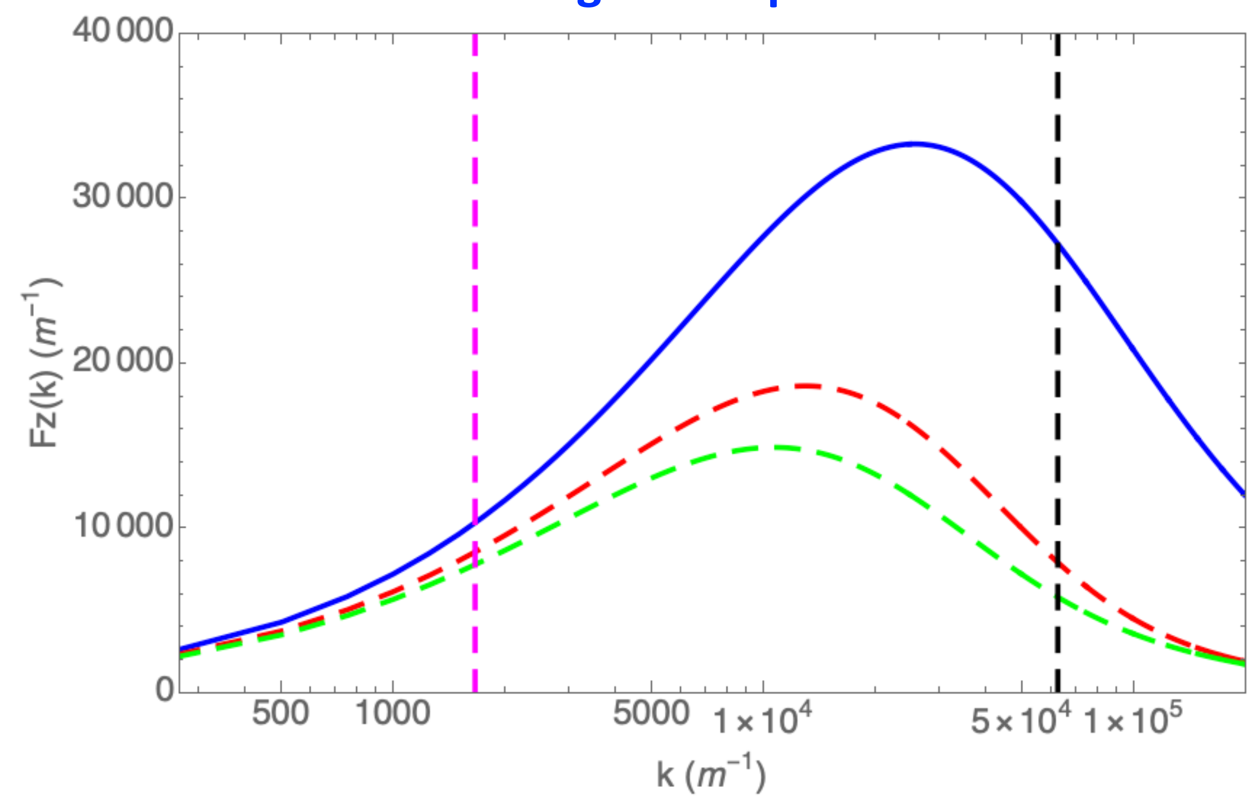
1. Impedance theory of SC

Test impedance models using cERL-FEL beam parameters

Beam parameters at POINTD:
σ_x=0.445 mm, σ_y=0.676 mm, σ_z=0.6 mm, γ=19.6075



Log-Linear plot



Longitudinal impedance using Eq.(23a) on page.7

1. Impedance theory of SC

Test impedance models using cERL-FEL beam parameters

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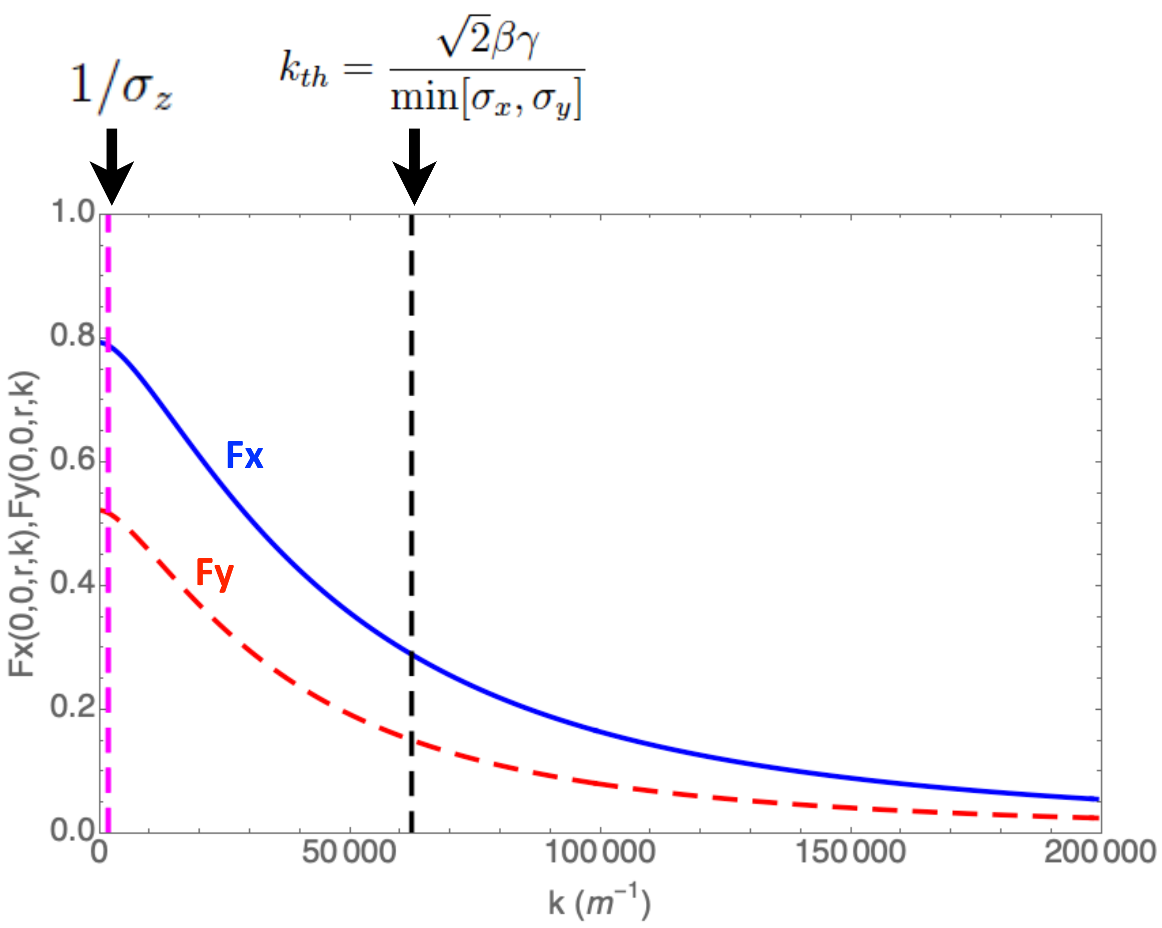
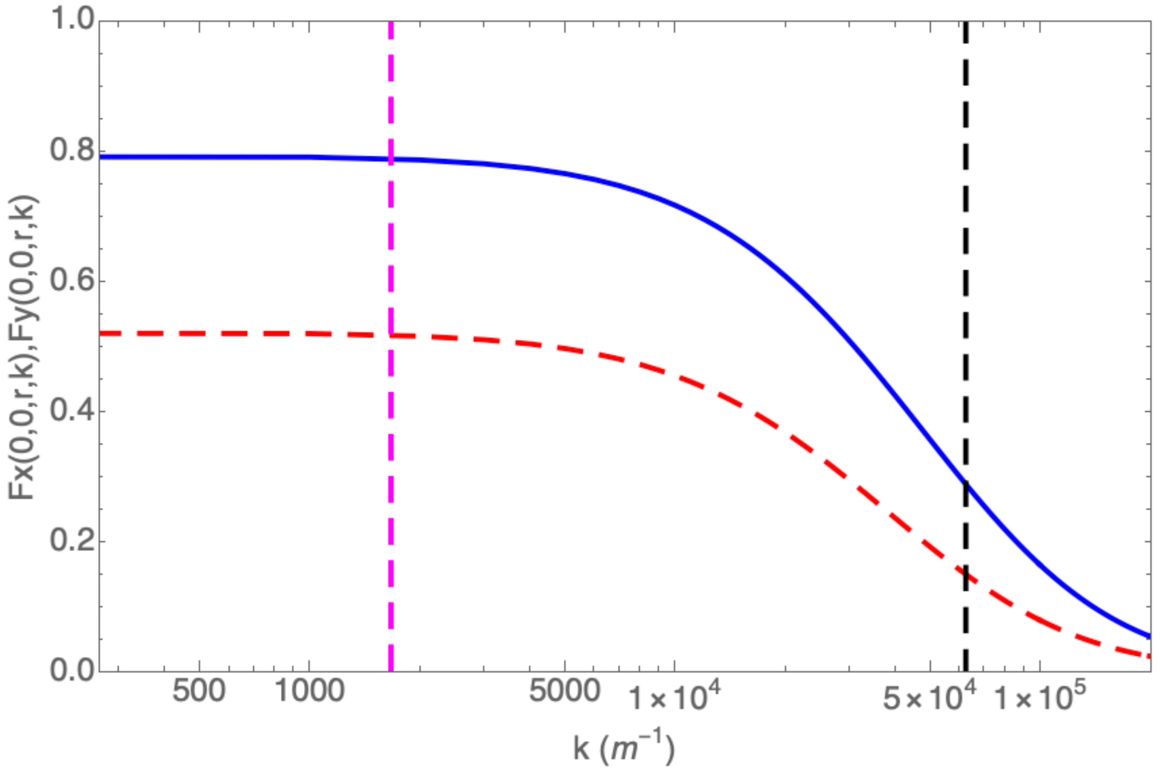


Log-Linear plot



On-axis transverse impedance using Eqs.(23b) and (23c) on page.7

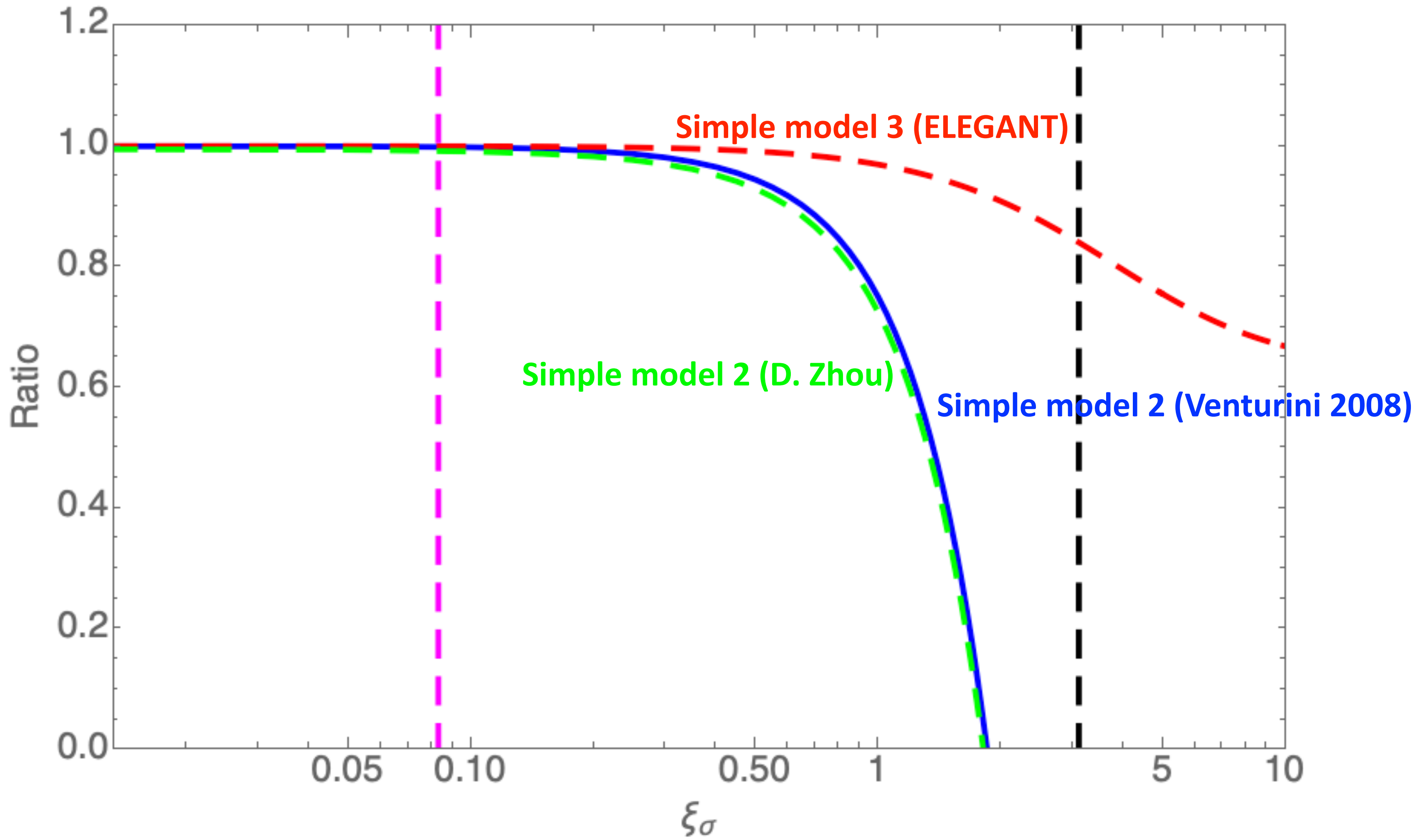
1. Impedance theory of SC

Test impedance models using cERL-FEL beam parameters

Beam parameters at POINTD:
σ_x=0.445 mm, σ_y=0.676 mm, σ_z=0.6 mm, γ=19.6075

$$r_b \approx 1.747(\sigma_x + \sigma_y)/2.$$

$$kr_b/(\beta\gamma)$$



Compare simple 1D (on-axis) LSC models normalized by Eq. (23a)

2. Models for TSC and LSC

Compare ELEGANT, GPT and SAD

	TSC	LSC	Comment
ELEGANT	YES	YES	**TSC(3D) turned on through SCMULT, assuming Gaussian fitted beam sizes in x, y and z directions. Linear TSC is available (optics matching? LSC(1D) uses impedance model, assuming Gaussian distributions in x and y directions, arbitrary density in z direction.**
GPT	YES	YES	**3D self consistent(?)**
SAD	YES	NO(?)	**SAD's flag WSPAC turns on TSC. Linear model for optics matching. Nonlinear model (Eqs.(25) and p.10) for TSC kick with transverse beam sizes calculated from optics (given initial emittances and beta functions)**
SAD [DZ]	YES	YES	**TSC(3D) similar to ELEGANT's SCMULT, assuming Gaussian distributions in x and y directions, arbitrary density in z direction. LSC(1D) same as ELEGANT's LSCDRIFT.**

2. Models for TSC and LSC

Compare ELEGANT, GPT and SAD

From GPT User Manual Version 3.39:

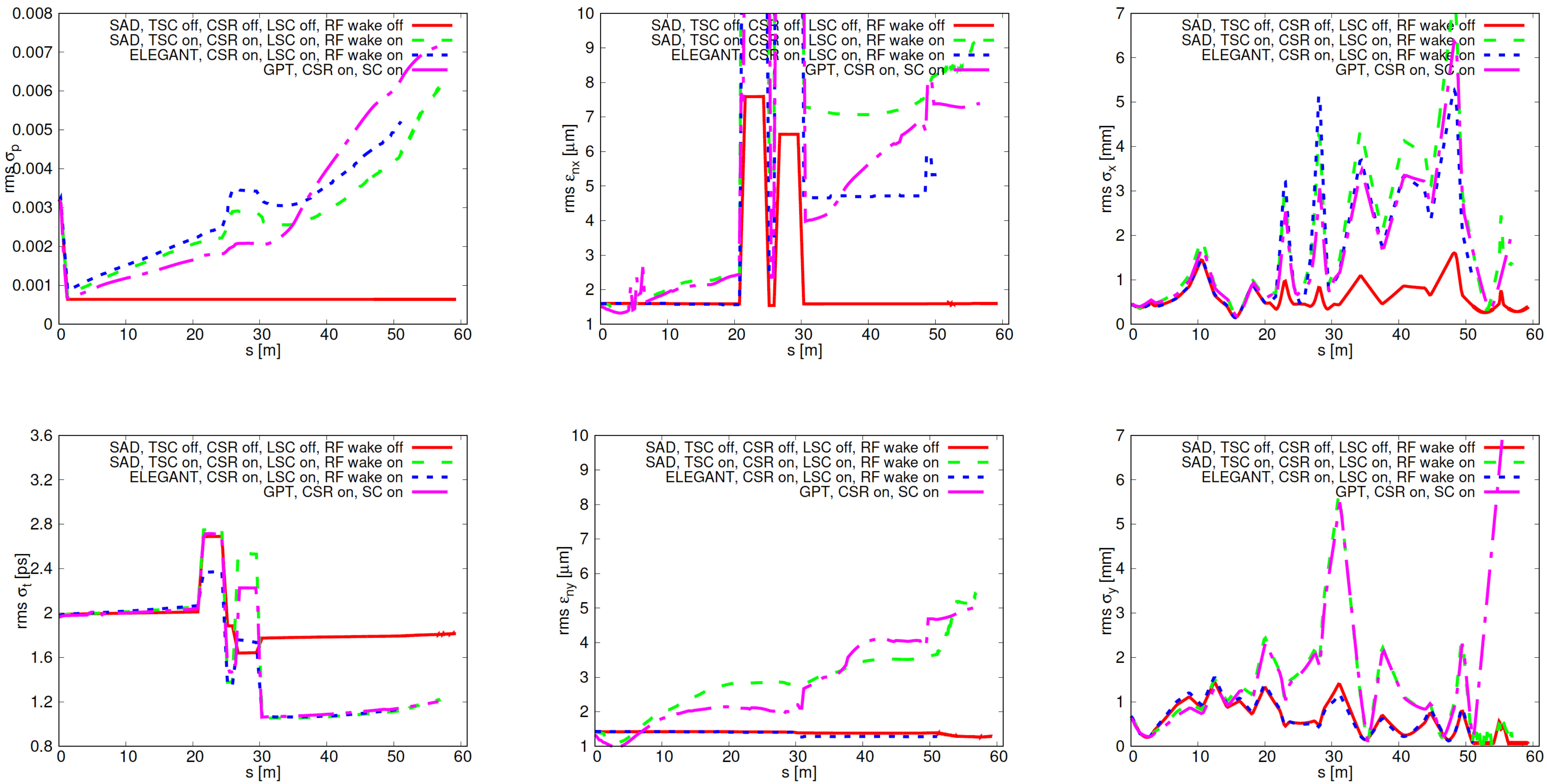
Table 1-B: Summary of all GPT space charge elements. Complexity is in terms of the number of particles *N*.

Name	Complexity	Granularity effects	Dim	Description
spacecharge3Dmesh	$O(N^{1.1})$	No	3D	PIC in rest frame
spacecharge3Dtree	$O(N \log N)$	Yes	3D	Barnes-Hut in rest frame
spacecharge3D	$O(N^2)$	Yes	3D	All pair-wise relativistic interactions
spacecharge3Dclassic	$O(N^2)$	Yes	3D	All pair-wise interactions
spacecharge2Dcircle	$O(N^2)$	No	2D	Cylindrically symmetric
Spacecharge2Dline	$O(N^2)$	No	2D	Continuous beam

2. Models for TSC and LSC

Compare ELEGANT, GPT and SAD: simulation results

The SC theories discussed in this talk may help understand the discrepancies?



Ref. D. Zhou, cERL-FEL meeting, Oct. 01, 2020, KEK

3. Summary and outlook

*** The SC theories are revisited**

** 3D impedance formulae are found with Gaussian bunches

** Conditions of simplifying the 3D formulae are found

** Consistent with the existing theories/models of SC

** Applicable conditions fo existing simple SC models are understood

*** Comments on SC models of ELEGANT, SAD and GPT**

** ELEGANT and SAD have similar models. These models can be improved from the viewpoint of the SC theories discussed in this talk

** Simulation results using GPT are still remarkably different from SAD. This should be well understood through careful benchmarks. For example:

*** Use well controlled examples such as very simple lattices

*** Use simple initial beam distributions

*** Use different options of SC models in GPT

*** Optics matching with SC**

** The linear TSC model is available in ELEGANT and SAD. It should be useful for the first and quick try of optics matching with SC.

** More accurate optics matching may need macro-particle tracking. The tracking results can be used to extract dynamic optics functions and then to optics matching.