Evolution of f-Divergence Between High-Dimensional Phase Space Distributions During Beam Transport

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August 17, 2026

Daejeon, Korea

Contents

Quantification of Beam Distribution Differences

- **Common Method:** Extract parameters from distributions for comparison.

$$\left.\begin{array}{l}\text{Mismatch Factor}\\ \text{RMS Emittance}\\ 99\,\%\ \text{Emittance}\end{array}\right\} \xrightarrow{\text{Shortcomings}}$$

  - Identical parameters do not guarantee identical distributions.
  - As the dimensionality increases, parameter comparison becomes more complex and less accurate.

- **Improved Method:** Directly compare the total distribution, We adopt

$$\boxed{f\text{-divergences.}}$$

  - Provide reasonable computational complexity.
  - Can obtain comprehensive difference information.

f-Divergences

- The f-divergences are a common class of methods used to measure the difference between two distributions, defined as follows:

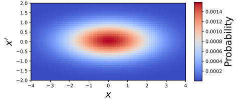
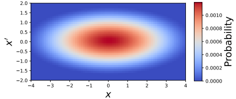
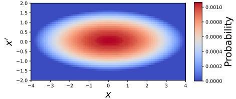
$$\boxed{D_f[\rho_1(\mathbf{x}) \parallel \rho_2(\mathbf{x})] = \int \rho_2(\mathbf{x})\, f\left[\frac{\rho_1(\mathbf{x})}{\rho_2(\mathbf{x})}\right] \mathrm{d}\mathbf{x},}$$

- $f(\cdot)$ is a convex function and satisfies $f(1) = 0$;
- Different $f(\cdot)$ correspond to different statistical divergences:

Name	$f(t)$	h	**Range**
Kullback-Leibler	$t \ln t$	$\rho_1(\mathbf{x}) \ln\left[\frac{\rho_1(\mathbf{x})}{\rho_2(\mathbf{x})}\right]$	$[0, \infty)$
Jensen-Shannon	$\frac{1}{2}\left[\ln\left(\frac{2}{t+1}\right)^{t+1} + t \ln t\right]$	$\frac{1}{2}\left\{\rho_2(\mathbf{x}) \ln\left[\frac{2\rho_2(\mathbf{x})}{\rho_1(\mathbf{x})+\rho_2(\mathbf{x})}\right] + \rho_1(\mathbf{x}) \ln\left[\frac{2\rho_1(\mathbf{x})}{\rho_1(\mathbf{x})+\rho_2(\mathbf{x})}\right]\right\}$	$[0, \ln 2]$
Total Variation	$\frac{1}{2}\lvert t-1\rvert$	$\frac{1}{2}\lvert\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\rvert$	$[0, 1]$
Squared Hellinger	$\frac{1}{2}(\sqrt{t}-1)^2$	$\frac{1}{2}\left[\sqrt{\rho_1(\mathbf{x})} - \sqrt{\rho_2(\mathbf{x})}\right]^2$	$[0, 1]$

Four forms of f-divergences; $t = \rho_1(\mathbf{x})/\rho_2(\mathbf{x})$*;* $h = \rho_2(\mathbf{x}) \cdot f[\rho_1(\mathbf{x})/\rho_2(\mathbf{x})]$*;* $\mathbf{x} \in \mathbb{R}^{2n}$

Several Common 4D Beam Distributions

Distribution with Elliptical Symmetry	**Definition** $\rho(x, x', y, y') = \rho(I)$ $I = \mathbf{x}^T \Sigma^{-1} \mathbf{x}$	**Schematic Diagram of 2D Projection** (x, x')
Gaussian	$\frac{1}{(\sqrt{2\pi})^4 \lvert\Sigma\rvert^{\frac{1}{2}}} \cdot e^{-\frac{1}{2} I}$	
Parabolic	$\frac{6}{(\sqrt{8\pi})^4 \lvert\Sigma\rvert^{\frac{1}{2}}} \cdot \left(1 - \frac{I}{8}\right), \quad I < 8$	
Waterbag	$\frac{2}{(\sqrt{6\pi})^4 \lvert\Sigma\rvert^{\frac{1}{2}}}, \quad I < 6$	

Quadratic form expression of beam distributions with elliptical symmetry; $\mathbf{x} = (x, x', y, y')^T$;
Σ *is a covariance matrix composed of 10 independent second-order moments;*
The above distributions can be uniformly written as $\rho(\vec{x}) = c \cdot \lvert\Sigma\rvert^{-\frac{1}{2}} \cdot g\left(\vec{x}^T \Sigma^{-1} \vec{x}\right)$

The f-Divergence Between Static Distribution

- **For distributions with the same covariance matrix Σ**, the f-divergence between them is fixed

$\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})$	D_{KL}	D_{JS}	D_{TV}	D_{Hel}
Parabolic – Gaussian	0.185837	0.054823	0.226909	0.262902
Waterbag – Gaussian	0.495922	0.134071	0.391299	0.407679
Waterbag – Parabolic	0.231856	0.071380	0.223872	0.309006

4D D_f between distributions with the same Σ

- **For uncoupled distributions:** the f-divergence corresponds to the mismatch factors (M_i) and emittance scaling factors (N_i).

$N_1 = N_2 = 1,\ M_1 = M_2 \rightarrow D_{f_1} = D_{f_2}$ $\quad$ $M_1 = M_2 = 0,\ N_1 = N_2 \rightarrow D_{f_1} = D_{f_2}$

Linear Beam Transport | Proof

f-Divergence remains invariant during linear transport.

$$\vec{x}_1 \longrightarrow \boxed{\vec{x}_2 = \mathbf{R}\vec{x}_1} \longrightarrow \vec{x}_2$$

Because of $\vec{x}_1^T\Sigma_1^{-1}\vec{x}_1 = \vec{x}_2^T\Sigma_2^{-1}\vec{x}_2$, $|\Sigma_1| = |\mathbf{R}^{-1}|^2|\Sigma_2|$ and $\mathrm{d}\vec{x}_1 = |\mathbf{R}^{-1}|\mathrm{d}\vec{x}_2$,

$$D_f\left[\rho_1(\vec{x}_1)||\rho_2(\vec{x}_1)\right] = \int \rho_2(\vec{x}_1) f\left[\frac{\rho_1(\vec{x}_1)}{\rho_2(\vec{x}_1)}\right] \mathrm{d}\vec{x}_1 = D_f\left[\rho_1(\mathbf{R}^{-1}\vec{x}_2)||\rho_2(\mathbf{R}^{-1}\vec{x}_2)\right]$$

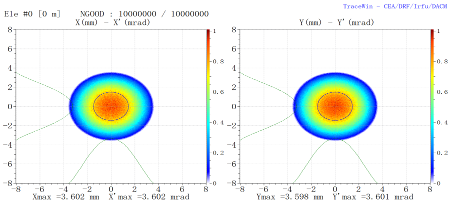
$$= \int c_2 \cdot |\mathbf{R}| \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_2\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right) \cdot f\left[\frac{c_1 \cdot |\mathbf{R}| \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_1\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right)}{c_2 \cdot |\mathbf{R}| \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_2\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right)}\right] \frac{1}{|\mathbf{R}|} \mathrm{d}\vec{x}_2$$

$$= \int c_2 \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_2\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right) \cdot f\left[\frac{c_1 \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_1\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right)}{c_2 \cdot |\Sigma_2|^{-\frac{1}{2}} \cdot g_2\left(\vec{x}_2^T\Sigma_2^{-1}\vec{x}_2\right)}\right] \mathrm{d}\vec{x}_2$$

$$= \int \rho_2(\vec{x}_2) f\left[\frac{\rho_1(\vec{x}_2)}{\rho_2(\vec{x}_2)}\right] \mathrm{d}\vec{x}_2 = D_f\left[\rho_1(\vec{x}_2)||\rho_2(\vec{x}_2)\right]$$

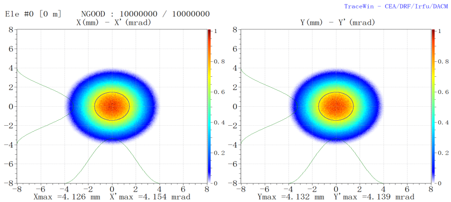
Linear Beam Transport | Simulation Verification

f-Divergence remains invariant during linear transport ($D_{f_1} = D_{f_2}$).

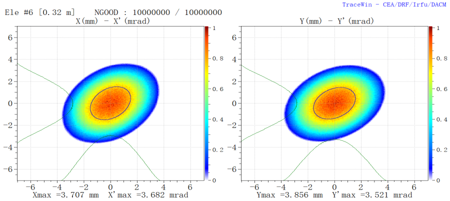


(a) Initial waterbag distribution

D_{f_1} $\longleftrightarrow$

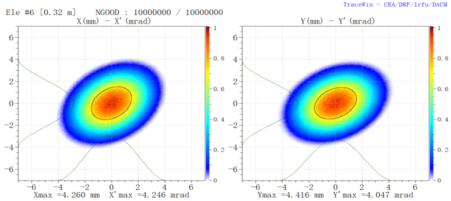


(b) Initial parabolic distribution



(c) Quadrupole transport (waterbag)

D_{f_2} $\longleftrightarrow$



(d) Quadrupole transport (parabolic)

Nonlinear Beam Transport | Proof

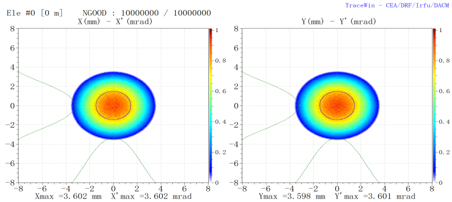
f-Divergence also remains invariant during nonlinear transport.

$$\vec{x}_1 \longrightarrow \boxed{\vec{x}_2 = h(\vec{x}_1)} \longrightarrow \vec{x}_2$$

$$\begin{aligned}
D_f[\rho_1(\vec{x}_2) \parallel \rho_2(\vec{x}_2)] &= \int \rho_2(\vec{x}_2) \cdot f\left[\frac{\rho_1(\vec{x}_2)}{\rho_2(\vec{x}_2)}\right] \mathrm{d}\vec{x}_2 \\
&= \int |J_{h^{-1}}(\vec{x}_2)| \cdot \rho_2\left[h^{-1}(\vec{x}_2)\right] \cdot f\left\{\frac{|J_{h^{-1}}(\vec{x}_2)| \cdot \rho_1\left[h^{-1}(\vec{x}_2)\right]}{|J_{h^{-1}}(\vec{x}_2)| \cdot \rho_2\left[h^{-1}(\vec{x}_2)\right]}\right\} \frac{1}{|J_{h^{-1}}(\vec{x}_2)|} \mathrm{d}\vec{x}_1 \\
&= \int \rho_2(\vec{x}_1) \cdot f\left[\frac{\rho_1(\vec{x}_1)}{\rho_2(\vec{x}_1)}\right] \mathrm{d}\vec{x}_1 = D_f[\rho_1(\vec{x}_1) \parallel \rho_2(\vec{x}_1)]
\end{aligned}$$

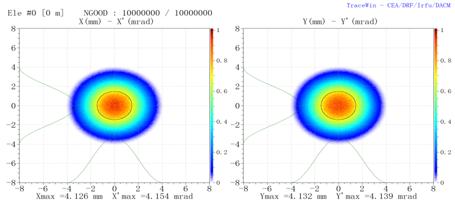
Nonlinear Beam Transport | Simulation Verification

f-Divergence also remains invariant during nonlinear transport $(D_{f_1} = D_{f_3})$.

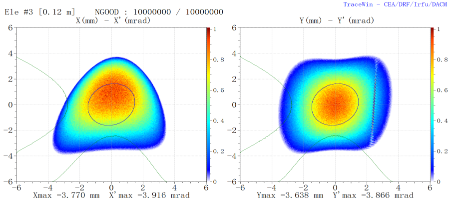


(e) Initial waterbag distribution

D_{f_1} $\longleftrightarrow$

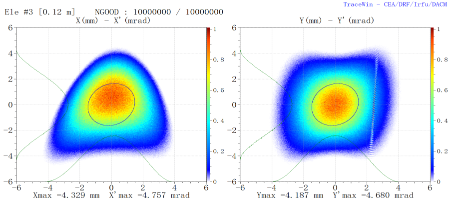


(f) Initial parabolic distribution



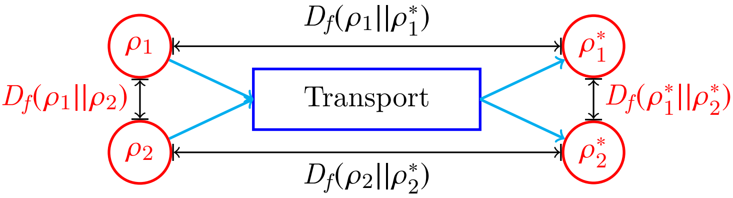
(g) Sextupole transport (waterbag)

D_{f_3} $\longleftrightarrow$



(h) Sextupole transport (parabolic)

Space Charge Forces



- Under linear and nonlinear transport: $D_f(\rho_1||\rho_2) = D_f(\rho_1^*||\rho_2^*)$.
- Space charge forces can break this conservation.
- Physical mechanism breaking conservation:
  - **Linear and nonlinear transport:** same map for all distributions;
  - **Space charge:** transport map becomes distribution-dependent.
- Application as a Diagnostic Tool:
  - Detecting SC-dominated regions, Quantifying space charge strength, ...
  - There is still much to explore about these properties.

Thanks for your attention!

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