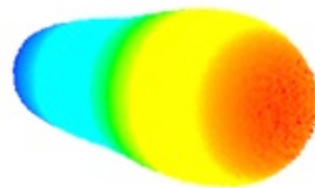


# Numerical modelling of photoemission for the PITZ photoinjector

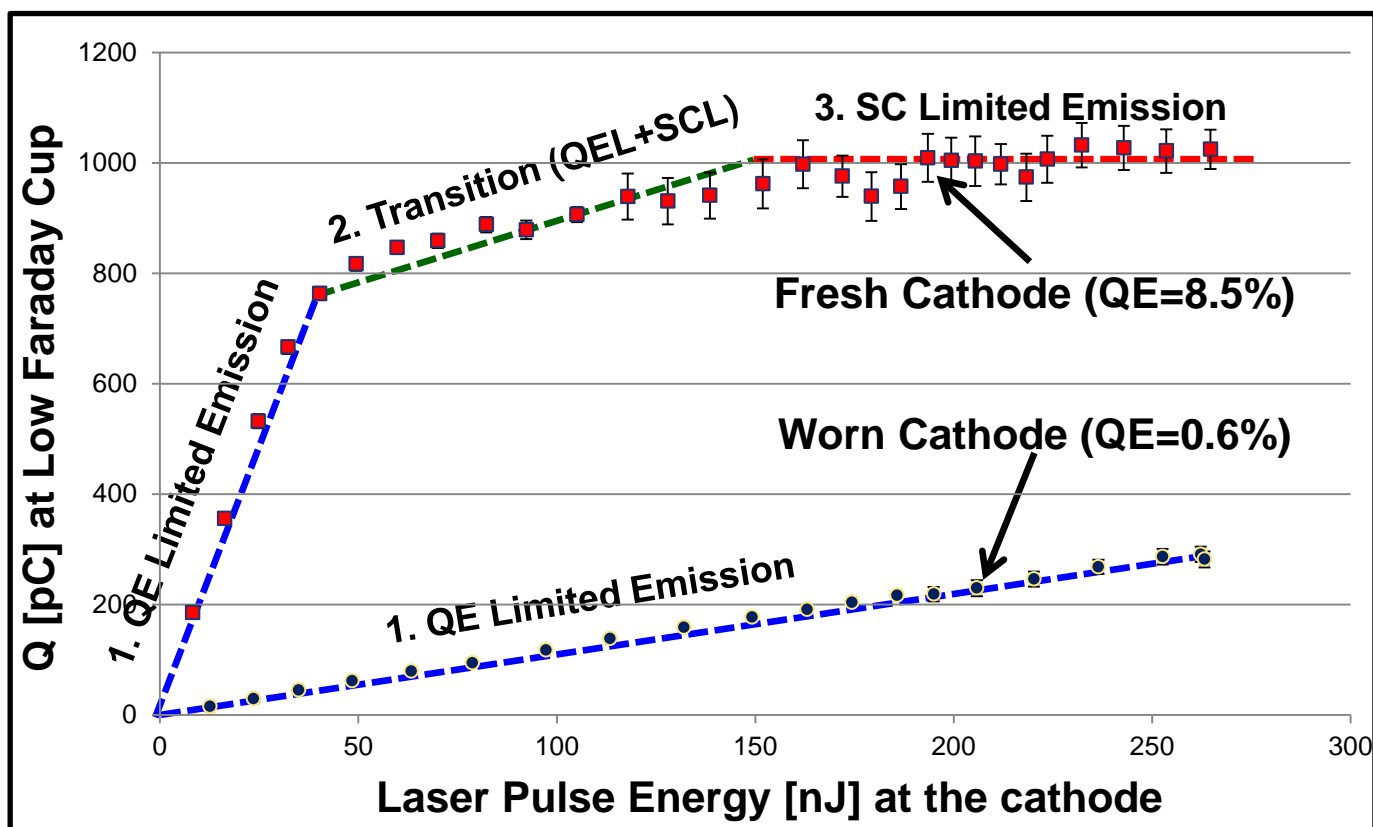


Ye Chen, Erion Gjonaj, Wolfgang Müller, Herbert De Gersem, Thomas Weiland  
TEMF, TU Darmstadt

**DESY-TEMF Collaboration Meeting**  
**DESY, Hamburg, June 15<sup>th</sup> 2015**



## Charge vs Laser Pulse Energy\* identified emission regimes for OLD and NEW cathodes



## Motivation

1. Identify source of discrepancies between measurement and simulation in terms of photoemission parameters.
2. Develop a numerical model of photoemission.

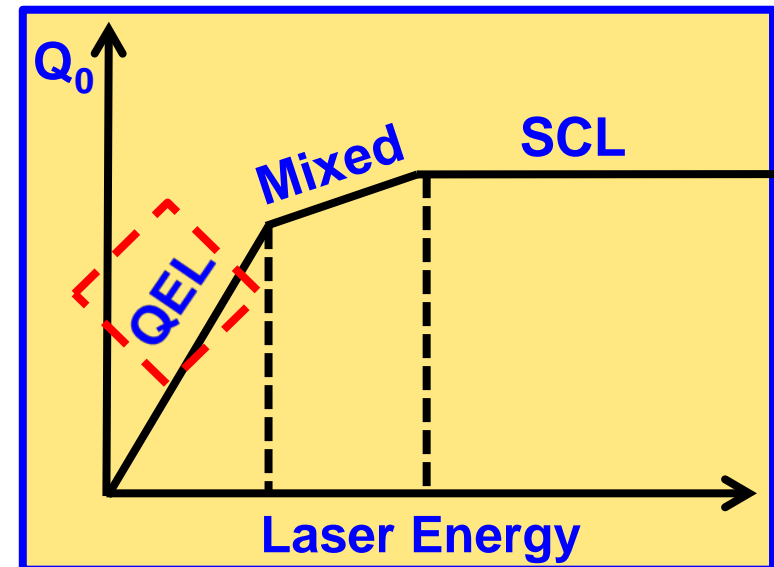
\*Measurement data sets provided by PITZ, 17.03.2015

- **Introduction**
- **Self-consistent QE limited bunch emission (QEL)**
  - Characterization of different photocathodes
  - Influences of Schottky effect on bunch temporal profile
- **Numerical modelling of space charge limitation (SCL)**
  - Methods and comparisons
  - Numerical issues
- **Summary & Perspective**
- **Discussions**

# Self-consistent QE limited bunch emission (QEL)

## QEL emission modelling

- $Q_{\text{tot}}$ 
  - i. Total bunch charge produced by the laser pulse at cathode
  - ii. Input bunch charge for simulation
- $E_{\text{tot}} \longrightarrow$  QE
  - i. Influences of Schottky effect on bunch temporal profile



Simulation assumption

# QEL bunch emission: key factors

- **Two related but independent processes:**
  1. **Charge production:** the **laser pulse** illuminates the **photocathode** and produces electrons at the cathode for extraction.
  2. **Charge (electrons) emission:** decisions of emission are made by the **local total field** at the cathode at the moment of extraction.
  
- **Key factors**
  1. **Laser pulse:** temporal shape and energy
  2. **Local fields at cathode:** RF+SC, perpendicular to the PEC surface
  3. **Quantum efficiency (QE) of photocathode**

# QEL bunch emission: relation between $E_{cath}$ , QE and $Q_{tot}$

## With no applied fields

$$QE^* = \eta [h\nu - \Phi_{cath0}]^2 \quad (1)$$

$\eta$ : cathode factor that depends on material properties such as the absorption coefficient, density of states, transition probability, and the angle of incidence of the laser light.

$h\nu$ : photon energy, 4.81 eV

$\Phi_{cath0}$ : work function with no applied field, 3.5 eV

$$Q_{tot} = e \frac{E_{laser}}{h\nu} QE \quad (2)$$

$$Q_{tot} = \int_{t_0}^t \iint_{xy} e \frac{P_{laser}(\tau)}{h\nu} QE(\eta; x, y, z = 0, \tau) dx dy d\tau \quad (6)$$

$$E_{cath}(x, y, z = 0, t)$$

work function correction due to field effects

$$\Delta\Phi(x, y, z = 0, t) = \sqrt{\frac{e^3}{4\pi\epsilon_0} E_{cath}(x, y, z = 0, t)} \quad (3)$$

$$\Phi_{cath} = \Phi_{cath0} \mp \Delta\Phi(x, y, z = 0, t) \quad (4) **$$

$$QE(\eta; x, y, z = 0, t) = \eta [h\nu - \Phi_{cath}]^2 \quad (5)$$

Local fields at cathode introduce space- and time- dependences to QE, while the latter corrects distributions of the emitted electron bunch accordingly.

\* QE: incident photon to converted electron (IPCE) ratio.

\*\* " $\mp$ " characterizes the work function variation when the total field changes sign.

# QEL bunch emission: modelling steps

- Total bunch charge produced at the cathode by the laser pulse:

$$Q_{tot} = \eta \int_{t_0}^t \iint_{xy} e \frac{P_{laser}(\tau)}{h\nu} \left[ h\nu - \left[ \Phi_{cath0} \mp \sqrt{\frac{e^3}{4\pi\epsilon_0} E_{cath}(x, y, z = 0, t)} \right] \right]^2 dx dy d\tau \quad (7)$$

- Modelling of  $Q_{tot}(\eta; x, y, z = 0, t)$

- **1<sup>st</sup> step: photocathode characterization**

- Determination of  $\eta$
    - Verification of  $\eta$  for different operation parameters (i.e.  $E_{laser}$ ,  $E_{cath}$ , temporal profiles)
    - Use determined  $\eta$  for Schottky effect investigations

- **2<sup>nd</sup> step: use determined  $\eta$  and full information of the local total fields at cathode to emit particles dynamically from the cathode**

- Dynamic corrections of transverse and longitudinal distributions of the emitted electron bunch within each time step

# Numerical approach

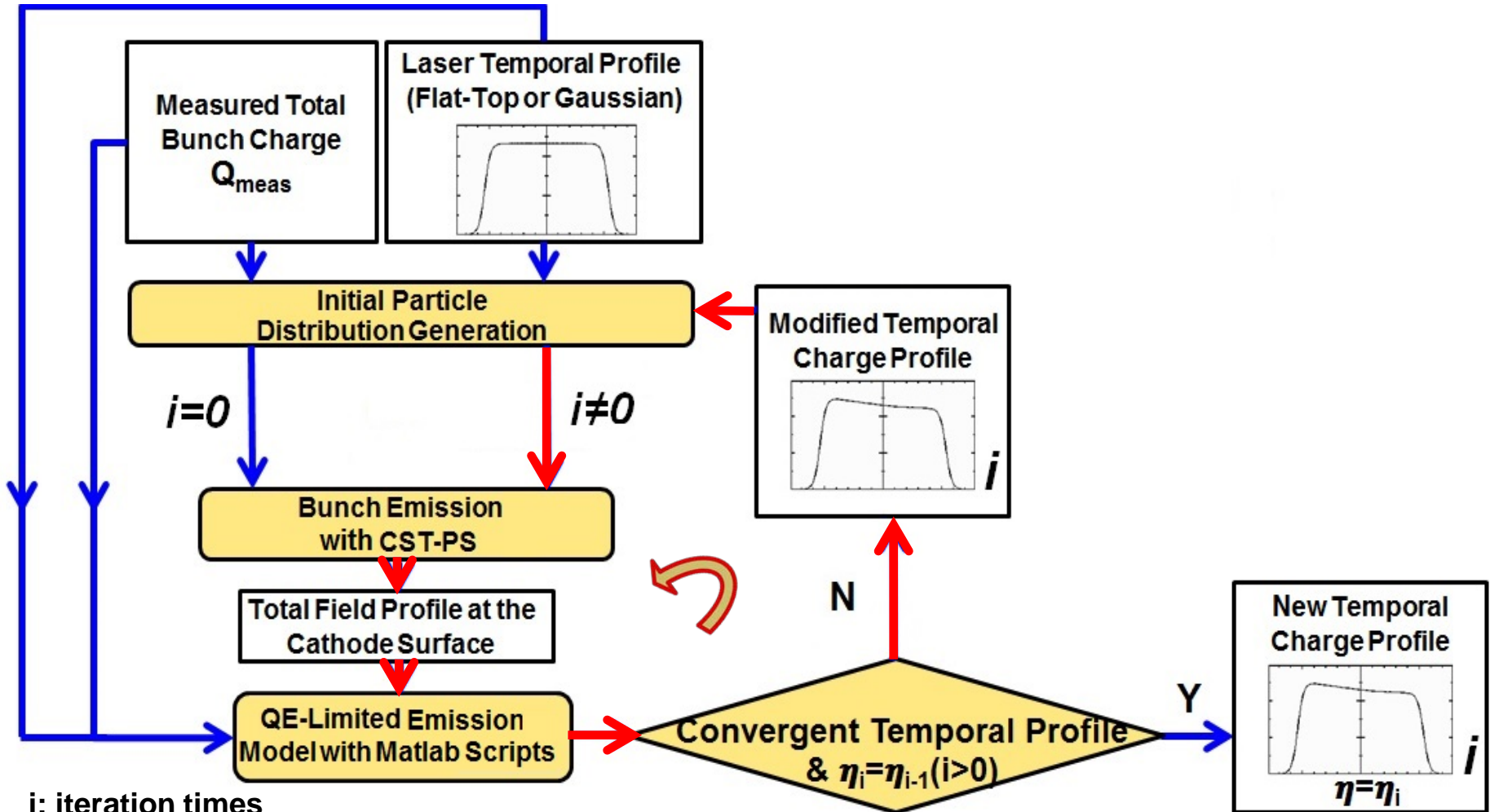
- Integrate equation (8) in a simulation loop, by correcting the temporal profile (TP) of the emitted electron bunch iteratively according to the local fields at cathode, such that  $Q_{tot}$  is normalized to  $Q_{meas}$  from measurements.

$$Q_{tot} = \eta \int_{t_0}^t e \frac{P_{laser}(\tau)}{h\nu} \left[ h\nu - \left[ \Phi_{cath0} \mp \sqrt{\frac{e^3}{4\pi\epsilon_0} E_{cath}(z=0, t)} \right]^2 \right] d\tau \quad (8)$$

- $E_{cath}$  is the total field (RF + SC) at the cathode, perpendicular to the surface.
- The transverse dependence of  $E_{cath}$  is not yet considered.
- Settings of initial particle distributions
  - Initial kinetic energy: 0.55 eV;
  - Transverse distribution ( $x, y, p_x, p_y$ ): uniform;
  - Temporal profile: laser pulse profile;
  - Momentum (angle) distribution ( $p_z$ ): isotropic;

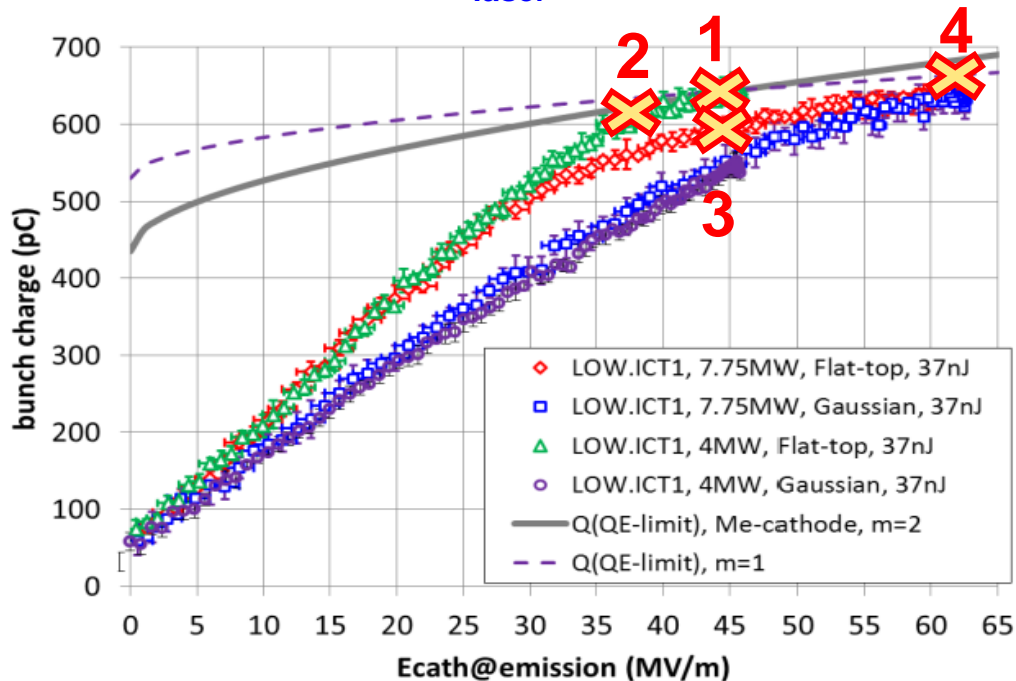


# Numerical approach



# Cathode (2013) characterization (1): determination of $\eta$ using different $E_{\text{cath}}$

\*Total bunch charge vs. gun gradient  
at  $E_{\text{laser}} = 37 \text{ nJ}$



## Results (1)

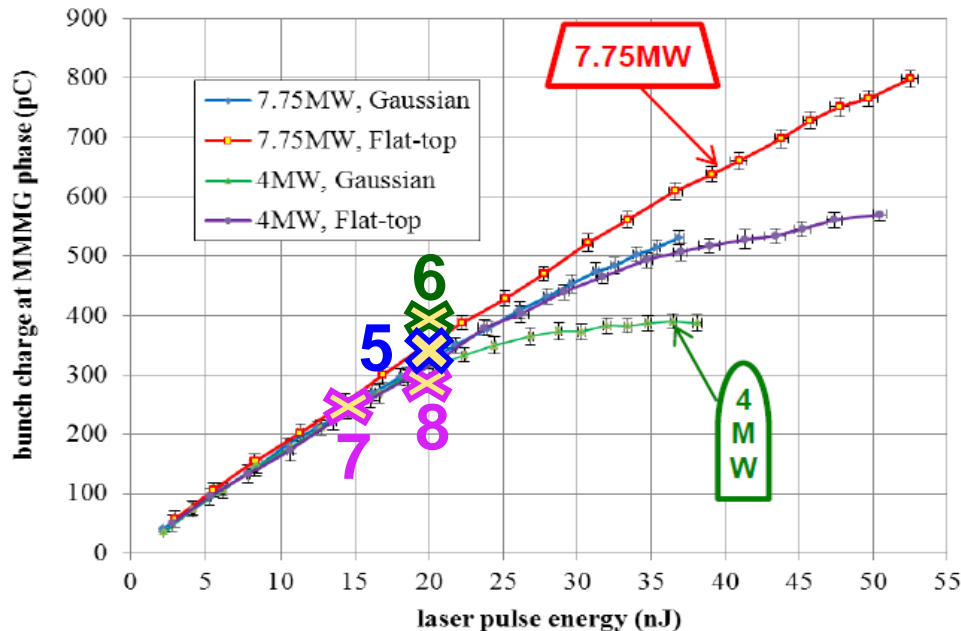
	$E_{\text{laser}}$ (nJ)	$E_{\text{cath}}$ (MV/m)	$\eta$	RF Power	TP
1	37	~46	0.0383	4 MW	FT
2		~36.7	0.0372	4 MW	FT
3		~46	0.0349	7 MW	FT
4		~63	0.0351	7 MW	FT

– Determined  $\eta$  is very close for the measurements using different cathode fields  $E_{\text{cath}}$ .

\* M. Krasilnikov, PIZ: Simulations versus  
Experiment, Darmstadt, 19.12.2013  
(measurement data sets taken from 02.2013)

# Cathode (2013) characterization (2): determination of $\eta$ using combinations of $E_{\text{laser}}$ / FT / GS / $P_{\text{rf}}$

\* Total bunch charge vs. laser pulse energy at MMMG phase



\* M. Krasilnikov, PITZ: Simulations versus Experiment, Darmstadt, 19.12.2013 (measurement data sets taken from 02.2013)

## Results (2)

	$E_{\text{laser}}$ (nJ)		$\eta$
5	20	FT + 4 MW	0.0357
6	20	FT + 7.75 MW	0.0361
7	15	Gaussian + 4 MW	0.0362
8	20	Gaussian + 4 MW	0.0340

– Determined  $\eta$  is also very close for the measurements using multiple combinations of machine parameters.

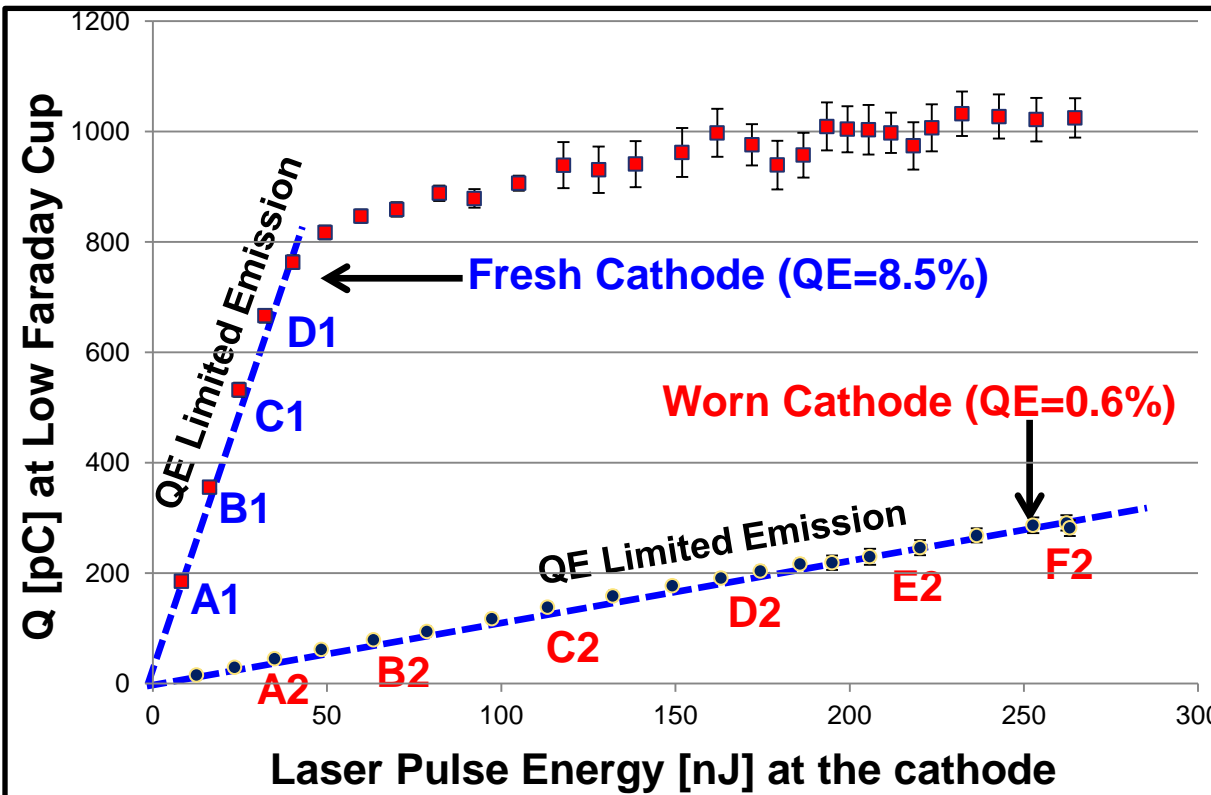
# Cathode (2015) characterization (3): determination of $\eta$ using different cathodes

New measurements\* in 2015

Bunch charge vs Laser Pulse Energy

Pgun=1.5 MW at X0-90 phase and BSA=1.8mm.

With fresh cathode (QE=8.5%) and worn cathode (QE=0.6%)



## Results (3)

### Fresh Cathode

	$E_{\text{laser}}$ (nJ)	$\eta$
A1	8.22	0.0477
B1	16.32	0.0456
C1	24.79	0.0448
D1	32.23	0.0432

### Worn Cathode

	$E_{\text{laser}}$ (nJ)	$\eta$
A2	34.96	0.002710
B2	63.35	0.002608
C2	113.34	0.002548
D2	163.08	0.002451
E2	205.81	0.002332
F2	252.65	0.002371

# Cathode characterization: verification of $\eta$

No.	Laser Profile	RF Power	$E_{\text{laser}}$	$\eta$
1	Flat-Top (FT)	4 MW	37 nJ	0.0383
2	FT	4 MW	37 nJ	0.0372
3	FT	7.75 MW	37 nJ	0.0349
4	FT	7.75 MW	37 nJ	0.0351
5	FT	4 MW	20 nJ	0.0357
6	FT	7.75 MW	20 nJ	0.0361
7	Gaussian (GS)	4 MW	15 nJ	0.0362
8	GS	4 MW	20 nJ	0.0340
9	GS	1.5 MW	8.22 nJ	0.0477
10			16.32 nJ	0.0456
11			24.79 nJ	0.0448
12			32.23 nJ	0.0432
13	GS	1.5 MW	34.96 nJ	0.002710
14			63.35 nJ	0.002608
15			113.34 nJ	0.002548
16			163.08 nJ	0.002451
17			205.81 nJ	0.002332
18			252.65 nJ	0.002371

**Cathode 1, 02. 2013**

$$\bar{\eta} \approx 0.0359$$

$$\frac{\eta_i - \bar{\eta}}{\eta_i} \times 100 < 6\%$$

**Cathode 2, 02. 2015**

$$\bar{\eta} \approx 0.0453$$

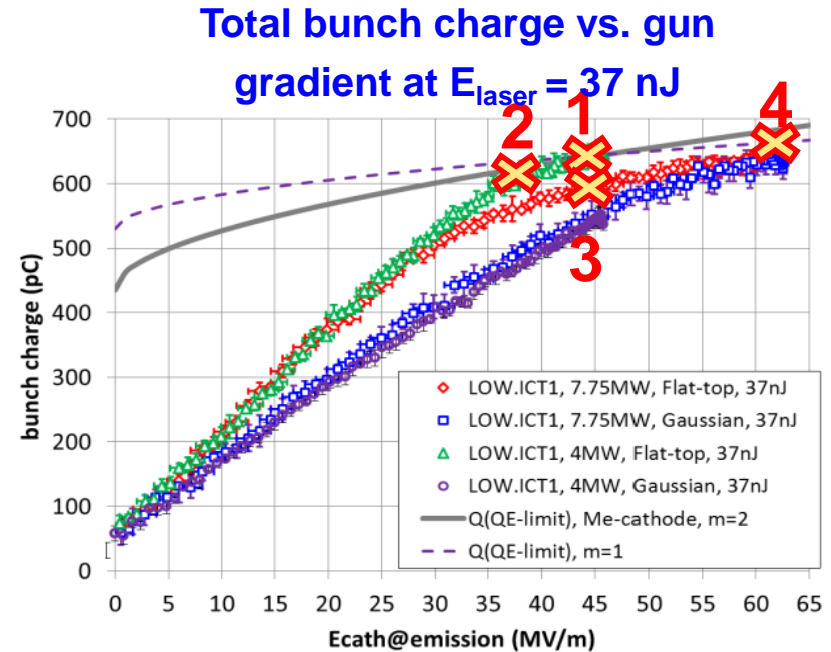
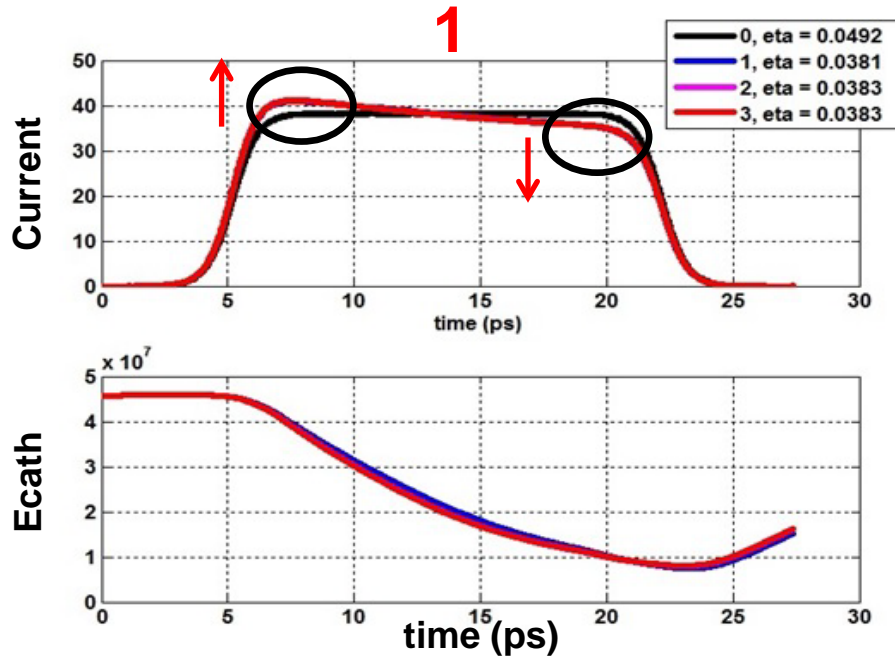
$$\frac{\eta_i - \bar{\eta}}{\eta_i} \times 100 < 5\%$$

**Cathode 3, 02. 2015**

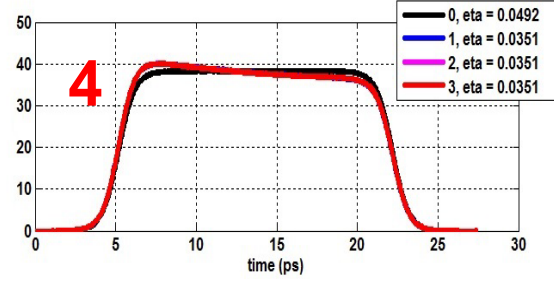
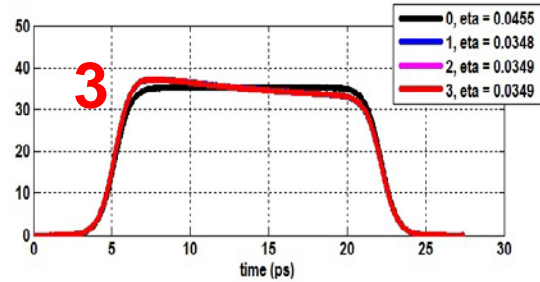
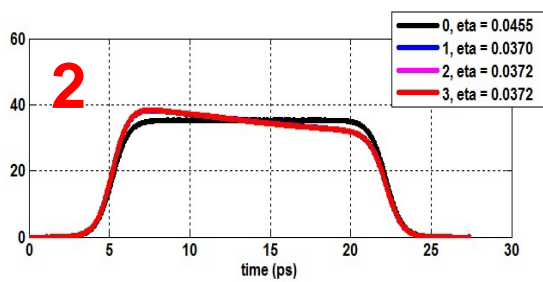
$$\bar{\eta} \approx 0.002503$$

$$\frac{\eta_i - \bar{\eta}}{\eta_i} \times 100 < 7\%$$

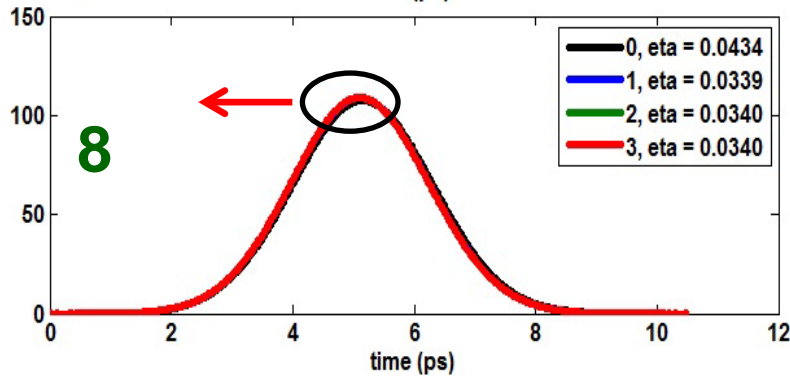
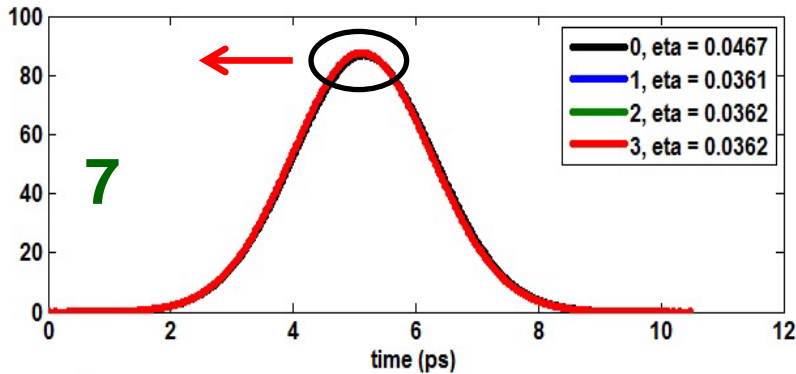
# Influence of Schottky effect due to $\eta$ (1)



- Schottky effect brings asymmetry to bunch temporal profile.
- It modifies the work function and thus corrects QE of cathode.

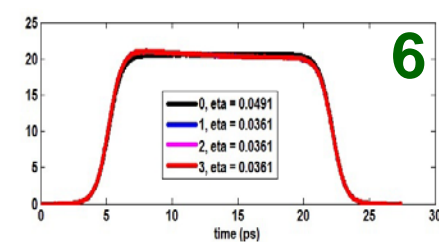
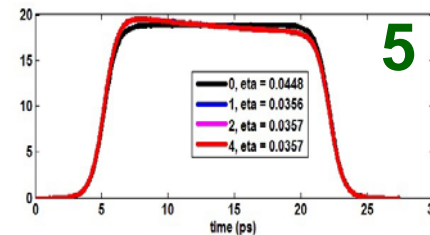
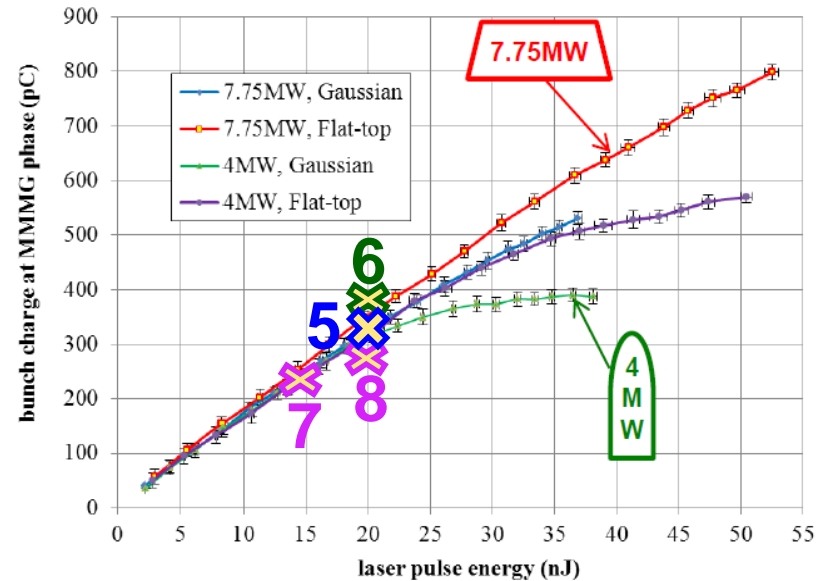


# Influence of Schottky effect due to $\eta$ (2)



- Temporal profile "peak" shifts to earlier times.
- Effect not prominent.

## Total bunch charge vs. laser pulse energy at MMMG phase



# Intermediate summary

1. **QEL emission model proposed and fits well the measurement data.**
2. **Cathode characterizations done for 3 cathodes, cathode factor  $\eta$  determined using different machine operation parameters.**
3. **Predicted QE is comparable with the measurement data.**
  - i. "Worn cathode" : 0.54%~0.62% ; Measurement: ~0.6%
  - ii. "Fresh cathode" : 9.91%~10.98%; Measurement: ~8.5%

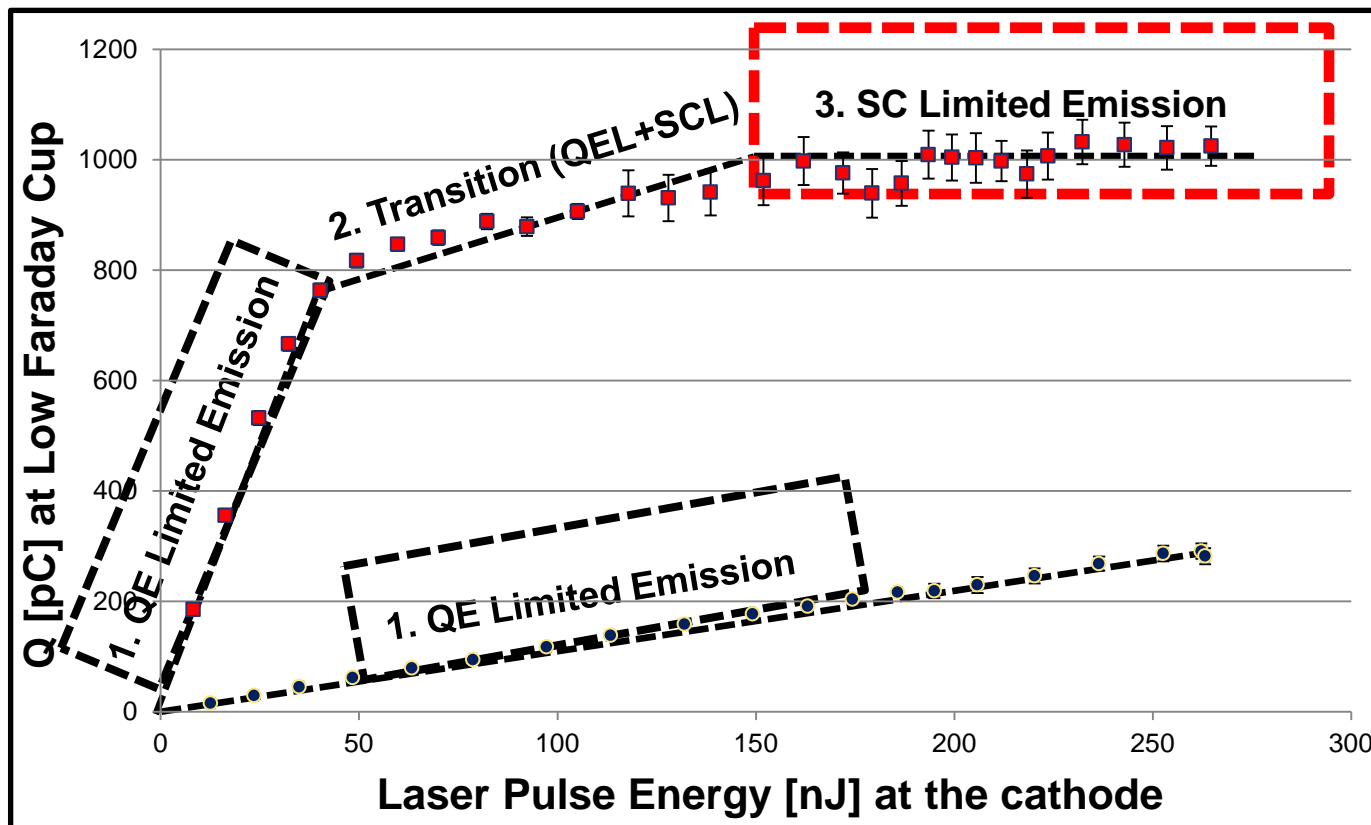
TABLE II. Various pr PITZ.	QE of cathode at PITZ *			INFN-LASA for use at	
Cathode #	Reflectivity at 543 nm	Cleaning process	Deposition date	QE at 254 nm	QE at 262 nm
58.1	56.9%	Standard	December 17, 2004	10.2%	...
34.6	56.5%	CO <sub>2</sub>	December 15, 2006	11.5%	7.5%
42.3	55.8%	Standard	April 5, 2007	11.5%	...
83.3 <sup>a</sup>	56.1%	CO <sub>2</sub>	December 22, 2006	12.0%	7.9%
90.1	56%	Standard	April 3, 2007	9.5%	...
109.1	57%	Standard	April 2, 2007	6.2%	...

\* F. Stephan et al., PRST-AB 13,  
020704 (2010)

4. **Influences of Schottky effect on emission using determined  $\eta$** 
  - i. Correcting bunch temporal profile: symmetry to asymmetry
  - ii. Emission peak shifts to earlier times; Effect not prominent.



# Numerical modelling of space charge limitation (SCL)



# Numerical modelling of SCL

- **Space charge limitation modelling method**
  - **"Brute-force"** (standard approach): very slow convergence, very expensive
  - **"Bunch charge iteration"**\* (speed-up technique): good convergence
- **Modelling status**
  - Both methods converge to the same SCL for FT-shaped bunches (FT).
  - Both methods agree with measurements for different machine parameters (FT).
  - Not applicable for GS-shaped bunches (GS).
- **Numerical modelling issues**
  - Convergence of the emitted bunch charge at / above SCL\*
  - Deviation in bunch charge prediction between different solvers\*\*

\* Y. Chen et al., Photoemission Studies for PITZ, DESY-Zeuthen site, 28.05.2014

\*\* E. Gjonaj, Emission Modeling for PITZ, DESY-Zeuthen site, 19.12.2013

# "Brute-force" method

## ▪ Definitions

- $Q_b$  : input bunch charge
- $Q_0$  : output bunch charge

## ▪ "Brute-force" technique

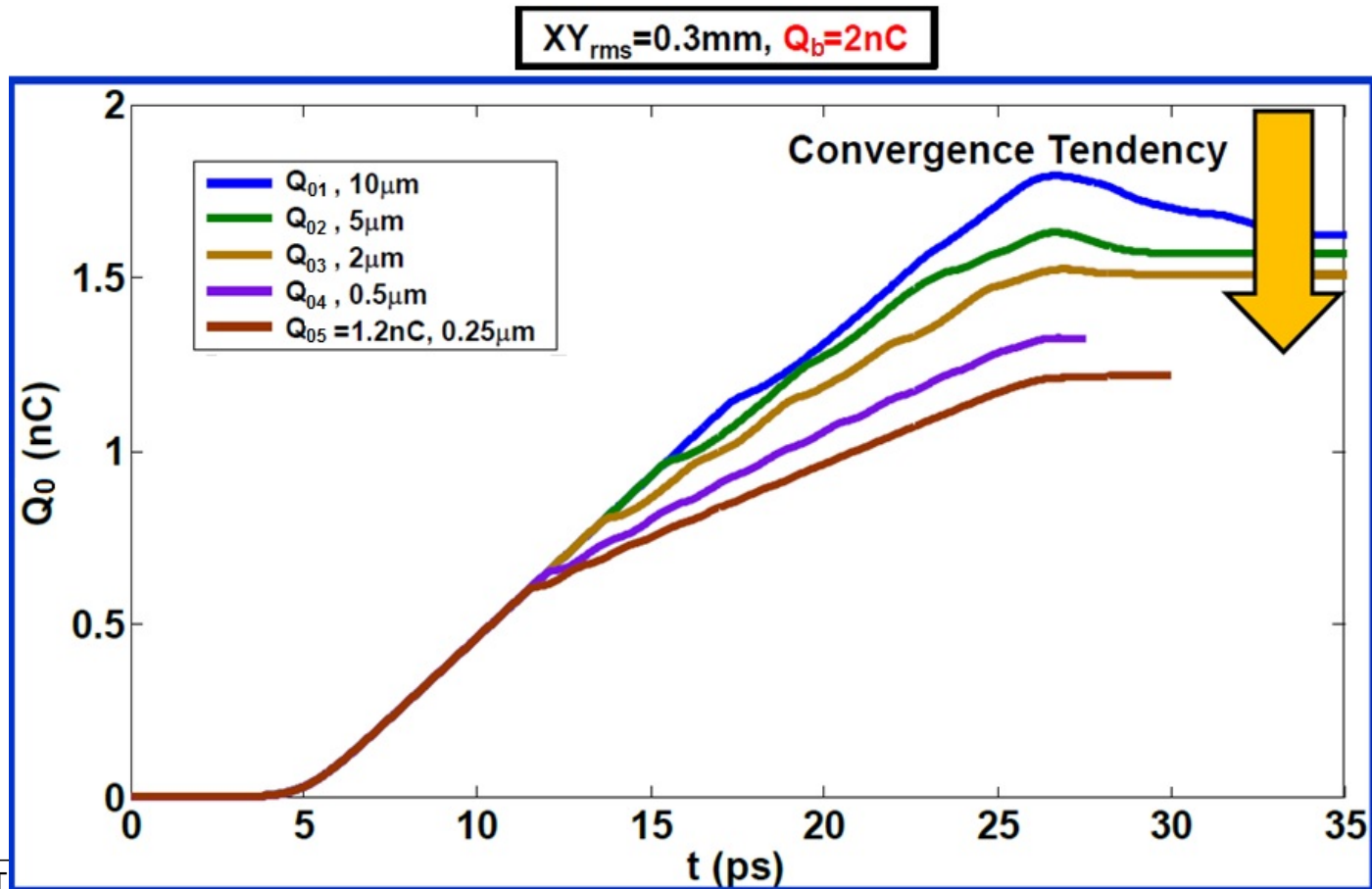
- Inject particles at the cathode, and estimate from the local fields whether they can be emitted or not.
- Convergence check needed.

## ▪ **Convergence of $Q_0$**

- w.r.t. mesh resolution ( $\Delta x, \Delta y, \Delta z$ )
- w.r.t. number of particles ( $N_p$ )
- w.r.t. time step ( $\Delta t$ )
- w.r.t.  $Q_b$

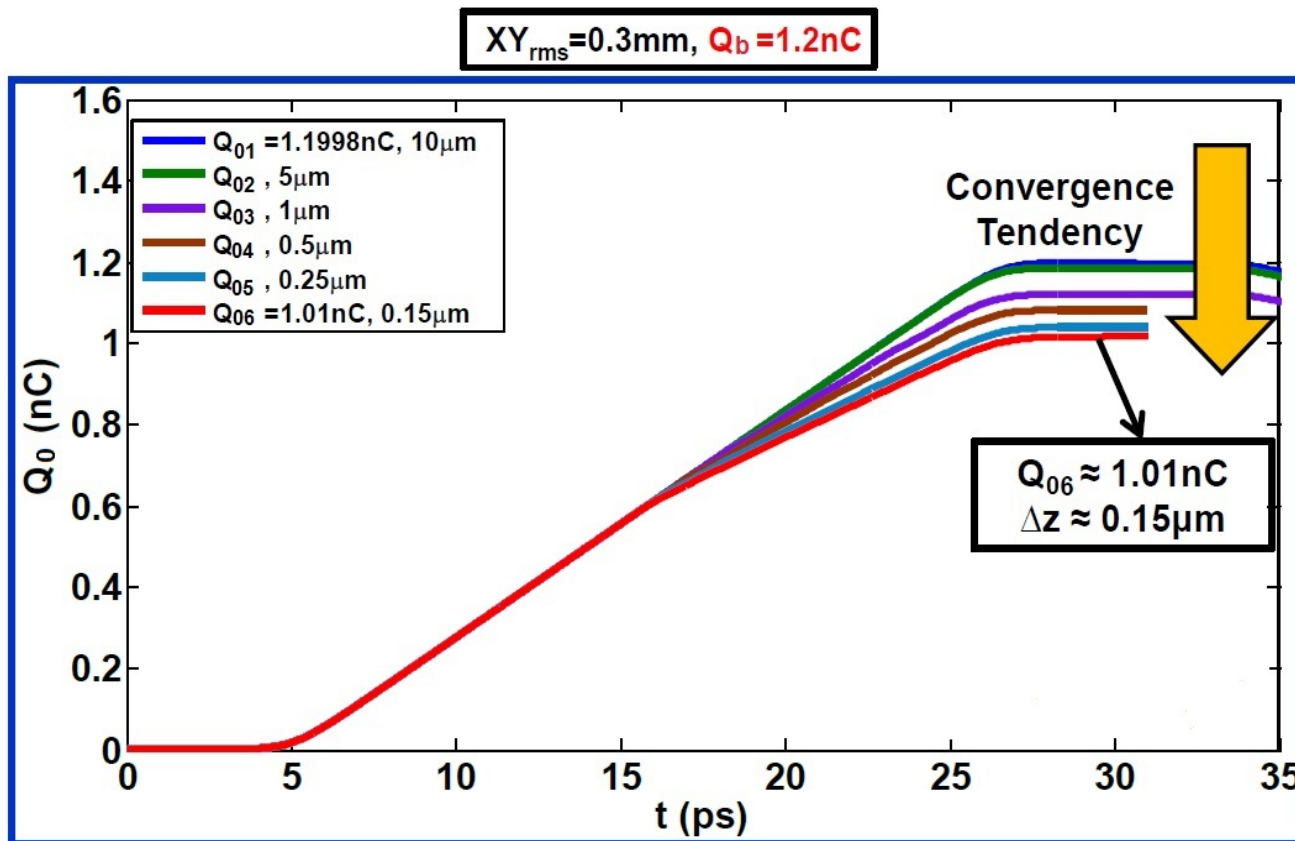
# "Brute-force" method: $Q_0$ w.r.t. mesh: flat-top-shaped bunch

- (0) Space charge limit **close to 1 nC** for the nominal bunch (measurement).
- (1) When  $Q_b \gg Q_0$ , numerical convergence w.r.t. mesh is rather slow (simulation).



# "Brute-force" method: $Q_0$ w.r.t. mesh: flat-top-shaped bunch

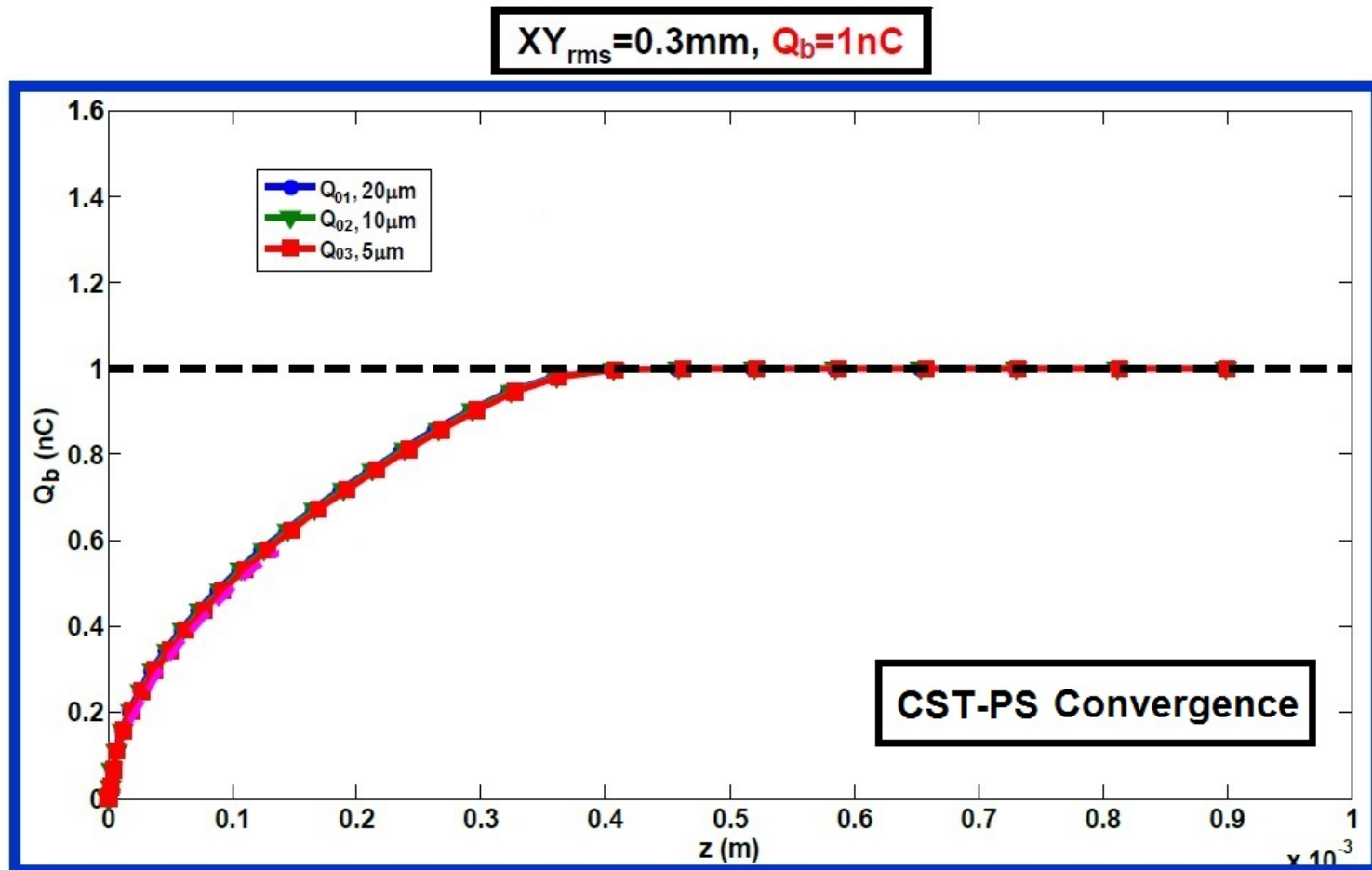
(2) As  $Q_b$  is approaching  $Q_0$ , the convergence w.r.t. mesh is getting better.



– The "brute-force" method can predict the space charge limit using a very fine mesh resolution, however, slow and expensive.

# "Brute-force" method: $Q_0$ w.r.t. mesh: flat-top-shaped bunch

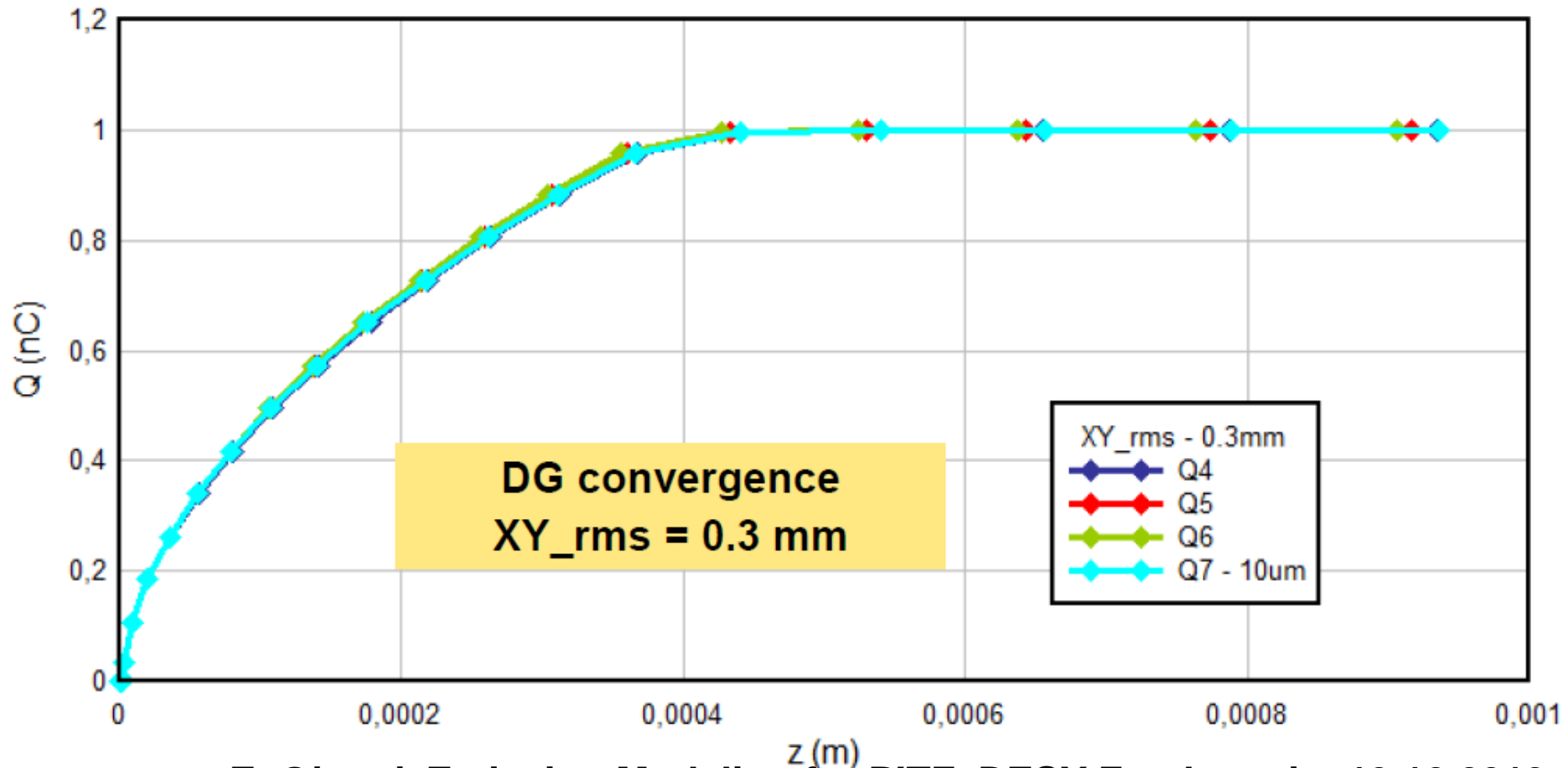
(3) When  $Q_b \approx Q_0$ , the convergence w.r.t. mesh is good.



# "Brute-force" method:

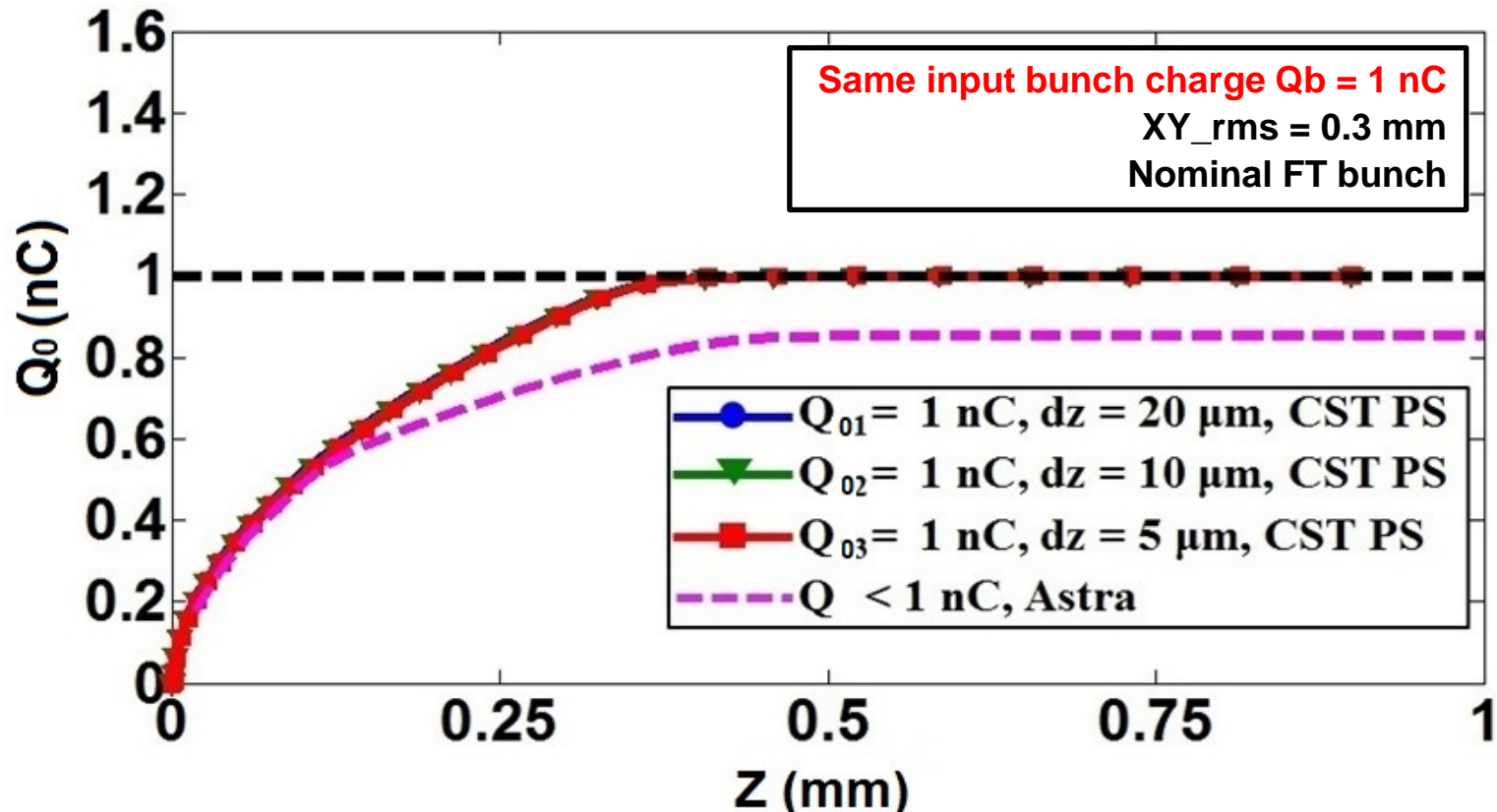
## $Q_0$ w.r.t. approximation order: flat-top-shaped bunch

(4) When  $Q_b \approx Q_0$ , the convergence w.r.t. approximation order is good.



E. Gjonaj, Emission Modeling for PITZ, DESY-Zeuthen site, 19.12.2013

# Deviation of SCL between different solvers



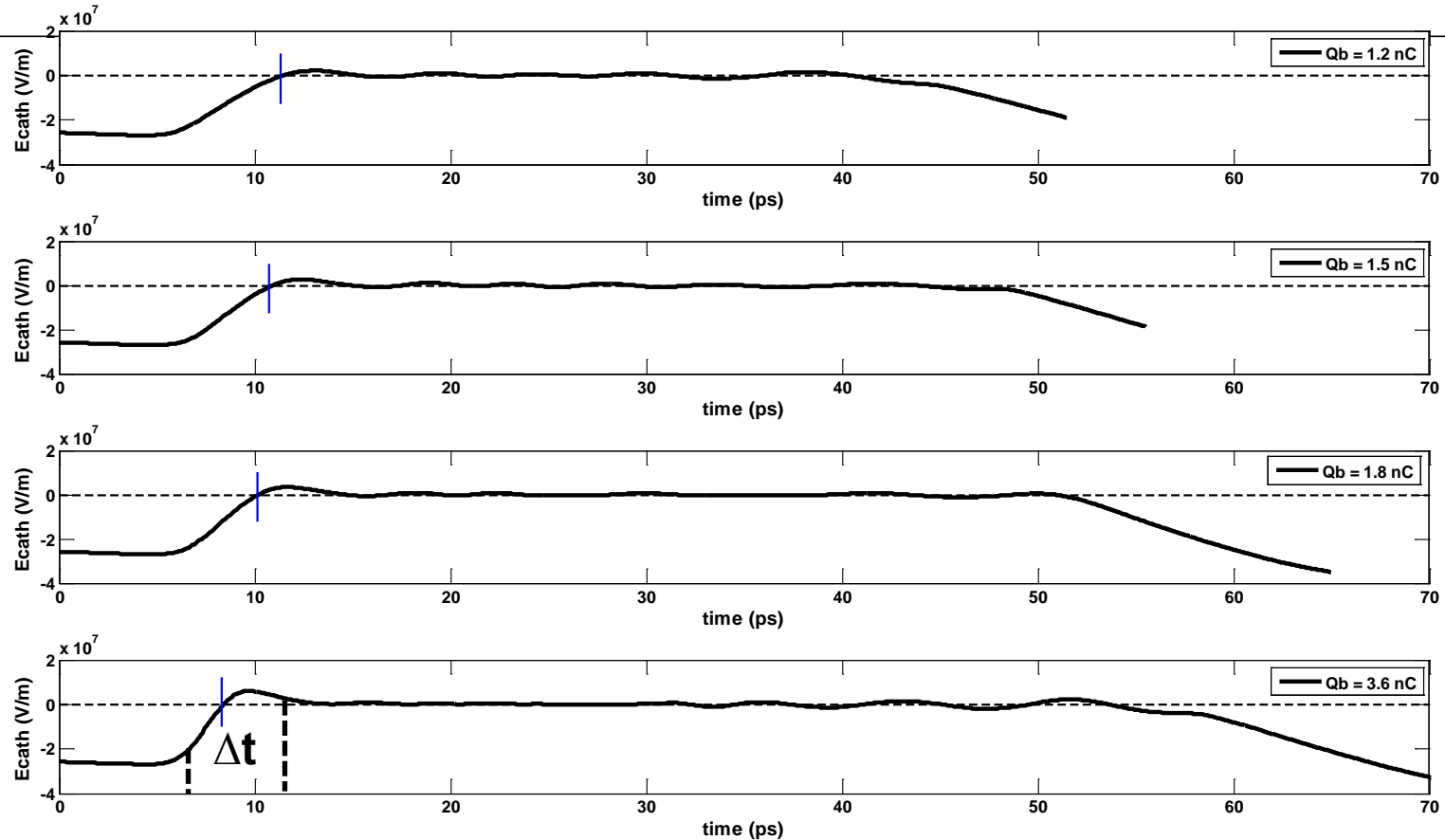
- Same input  $Q_b = 1 \text{ nC}$  for both algorithm.
- Calculations of SCL with standard approach (No Iteration)
- Different output  $Q_0$



# Motivation of "charge iteration method"



TECHNISCHE  
UNIVERSITÄT  
DARMSTADT

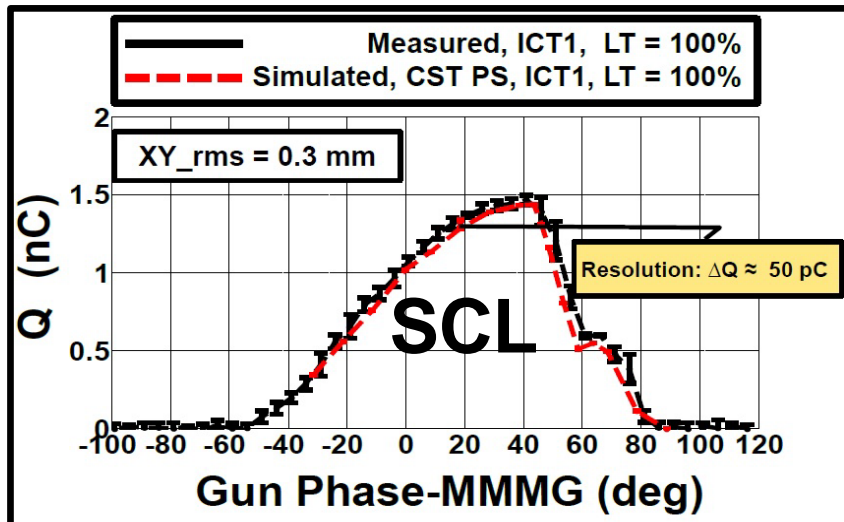


1. Space charge limit (SCL) occurs when the total field at the cathode changes sign.
2. Above SCL, this happens soon as the emission begins, meaning  $\Delta t \ll t$ .
3. During the beginning time of  $\Delta t$ , the steady state assumption is not valid, however, this method can still estimate from most of time in the emission process.

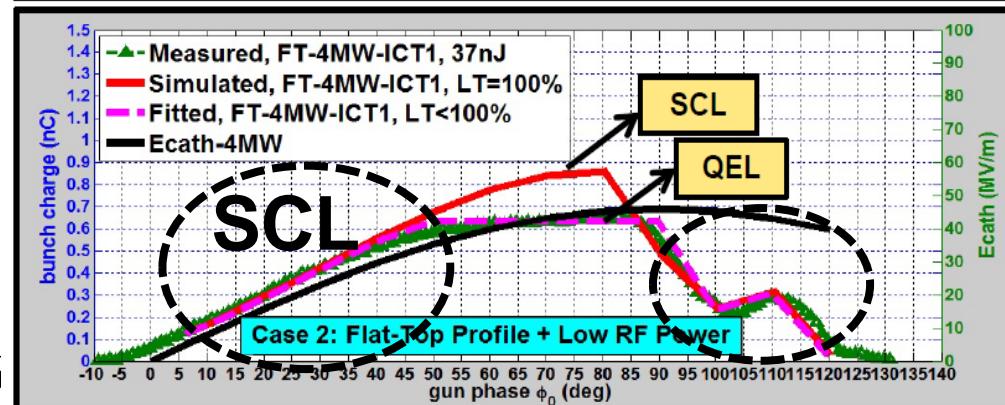
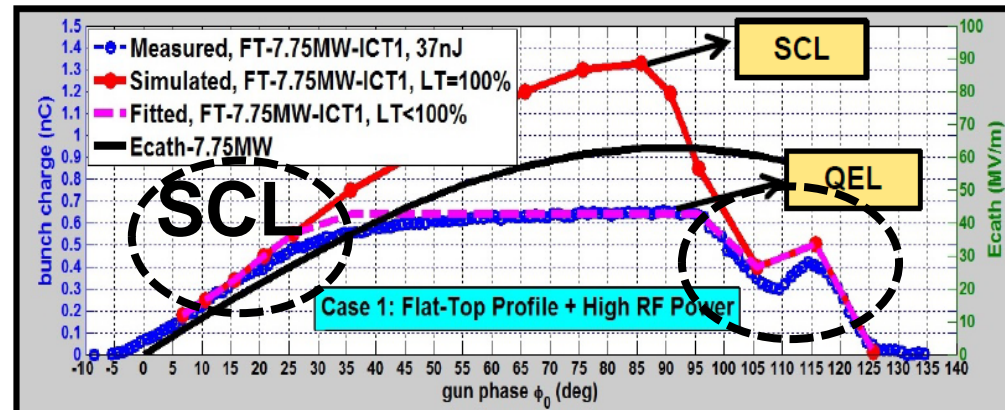
# Comparisons with measurements

- Using the charge iteration method, the simulated total bunch charges can well fit the measurement data under different experimental conditions in the case of FT-shaped bunches.

$XY_{rms} = 0.3 \text{ mm}$ ,  $Prf \approx 6 \text{ MW}$   
FT-shaped, 21.5 ps (FWHM)



$XY_{rms} = 0.3 \text{ mm}$ ,  $Prf \approx 7 \text{ MW}$  and  $4 \text{ MW}$   
FT-shaped, 17 ps (FWHM)



# Summary and Perspective

## 1. QE limited emission

- Model proposed
- Numerical approach used for three photocathode characterizations
- Determination of  $\eta$  verified under different experimental conditions
- Influences of Schottky effect investigated in terms of bunch temporal profiles

## 2. SCL modelling

- Numerical issues discussed w.r.t. convergence problem
- "Brute-force" agrees with "charge iteration" on SCL predictions
- Good agreements with measurements for FT-shaped bunches
- Method not valid for GS-shaped bunches

## 3. Perspective

- Implementation within each time step of corrections of the temporal and / or transverse distribution of the emitted bunch by using the full information of the local total fields at cathode
- New simulation tool preferable

*Thank you for your attention!*

*非常感谢您的关注!*