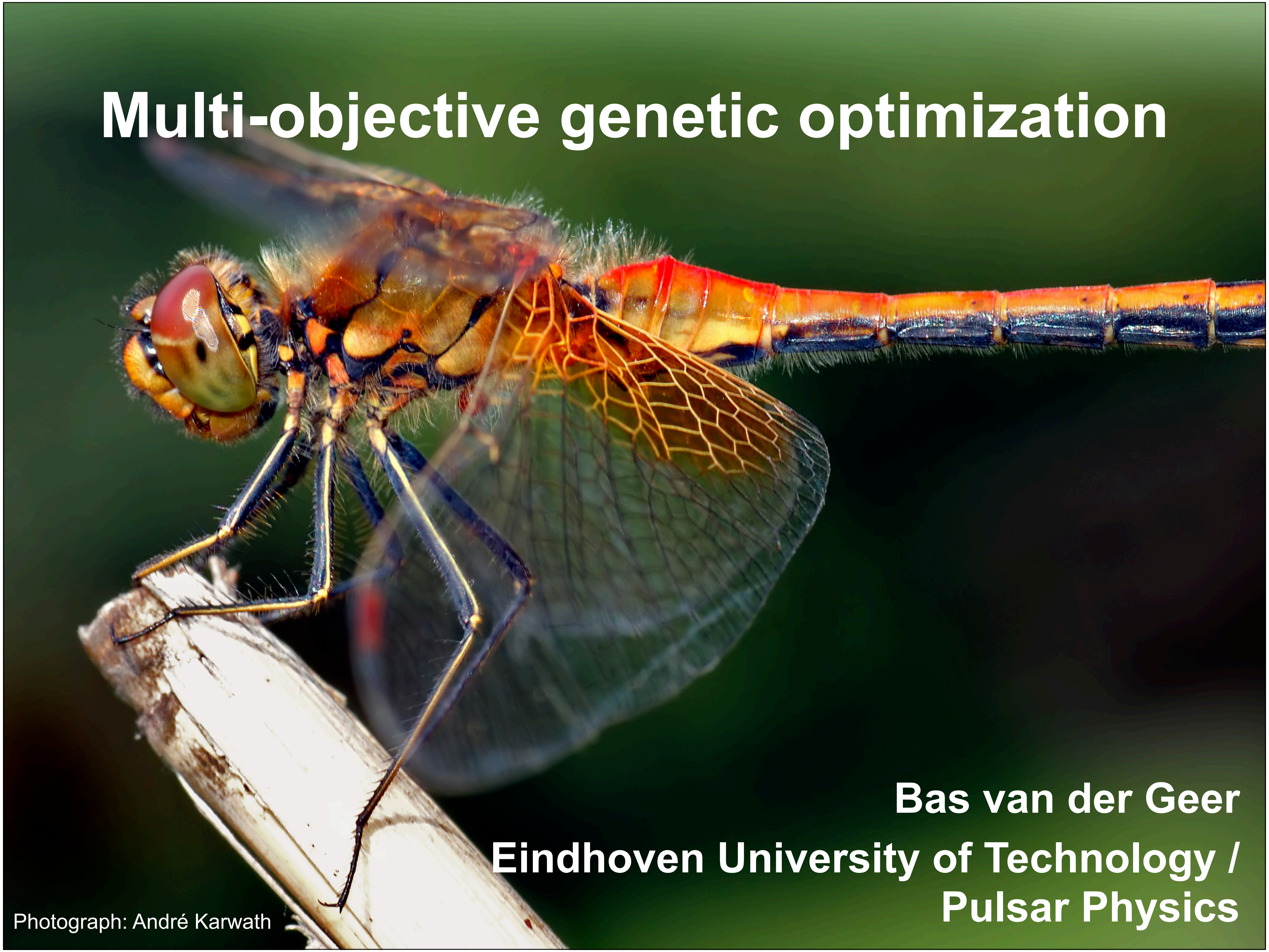

Multi-objective genetic optimization
Bas van der Geer
Eindhoven University of Technology /
Pulsar Physics
Photograph: André Karwath

Overview: We want it all…

Proven design

Top performance

Affordable

Overview: We want it all…

Top performance

Affordable

Overview: We want it all…

Affordable

Overview: We want it all…

Multi-objective optimization: Examples

Minimize weight *and* maximize strength

Maximize performance *and* minimize fuel consumption

Maximize profit *and* minimize risk

…

Kalyanmoy Deb et. al., A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II, IEEE Transactions On Evolutionary Computation, Vol. 6, No. 2, A

Multiple objectives: Beamline design

WE WANT IT ALL

- Typical objectives
  - High charge / current
  - Low emittance
  - Small spot size
  - Short pulse duration

- Variables
  - RF-phase / amplitude
  - Solenoid position / strength
  - Electrode geometry
  - Emission process (size, charge)

WE WANT IT NOW

- Time = money

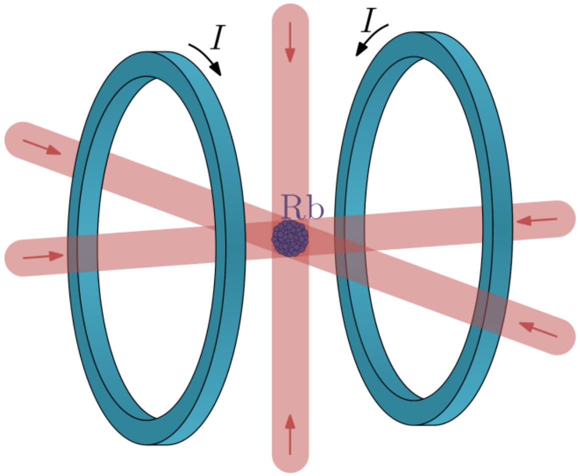
Transform to single objective: Bad idea

- Select a weight factor α_i for each objective function f_i
  - Minimize:

$$\boxed{F(a,b,c,d)=\alpha_1\ f_1(a,b,c,d) + \alpha_2\ f_2(a,b,c,d) + \ldots}$$

- Problems:
  - Requires tradeoffs to be made a-priori
    How much extra weight is equivalent to 10% stronger ?
  - Doesn't give tradeoff information
    How much stronger can we make it for 10% heavier ?

Ultracold Electron/Ion Source

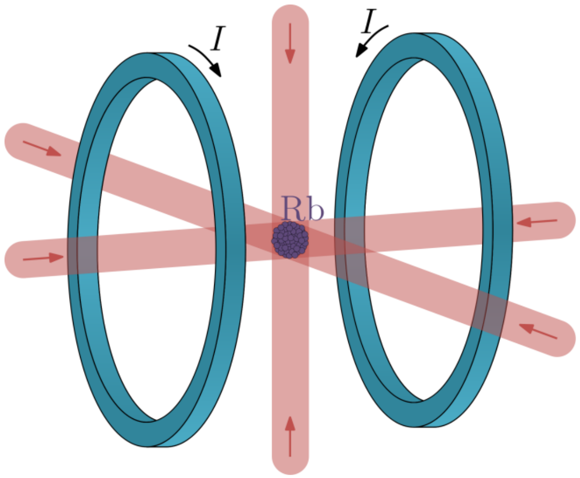


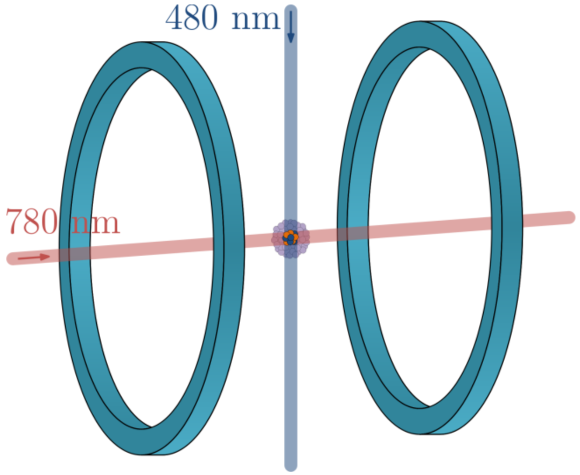
Trap & Cool

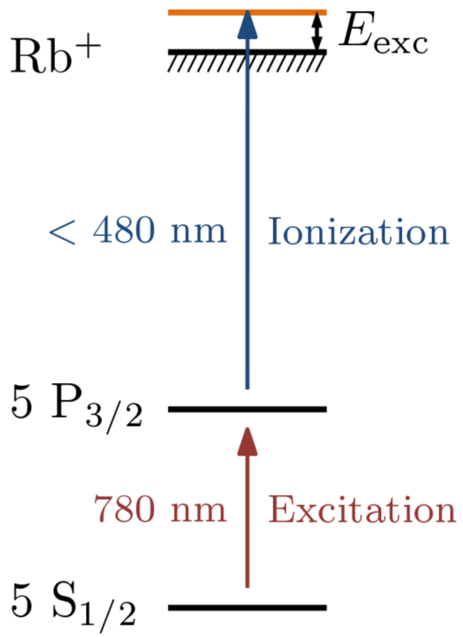
Magneto-optical trap

Density ≈ 10^{16} / m^3
RMS size ≈ 1 mm
T = 100 μK

Ultracold Electron/Ion Source







Trap & Cool

Magneto-optical trap

Density ≈ 10^{16} / m^3
RMS size ≈ 1 mm
T = 100 μK

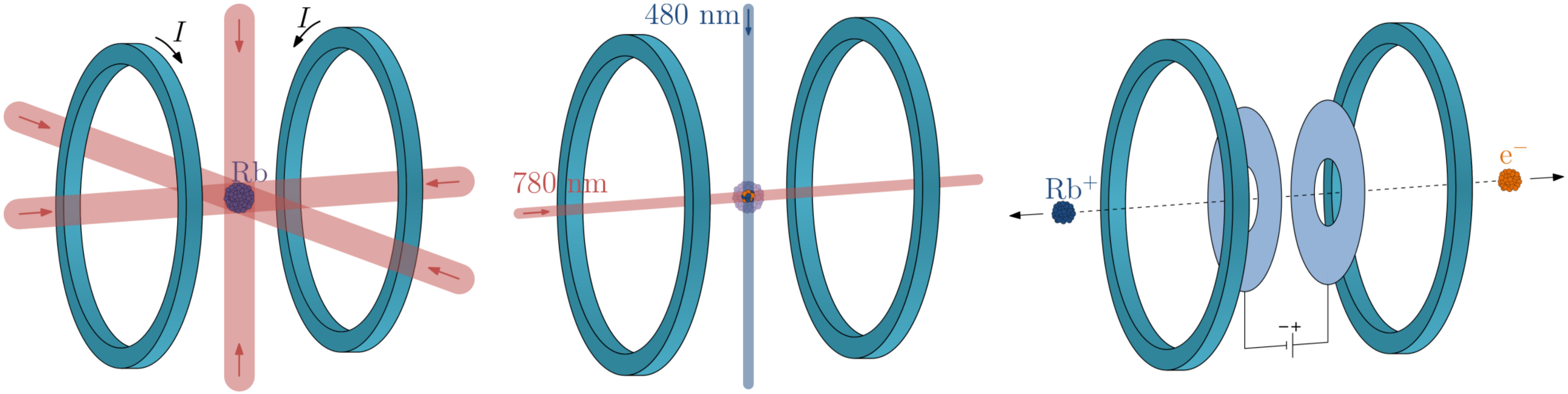
Ionize

Ultracold plasma

Ionization radius ≈ 50 μm

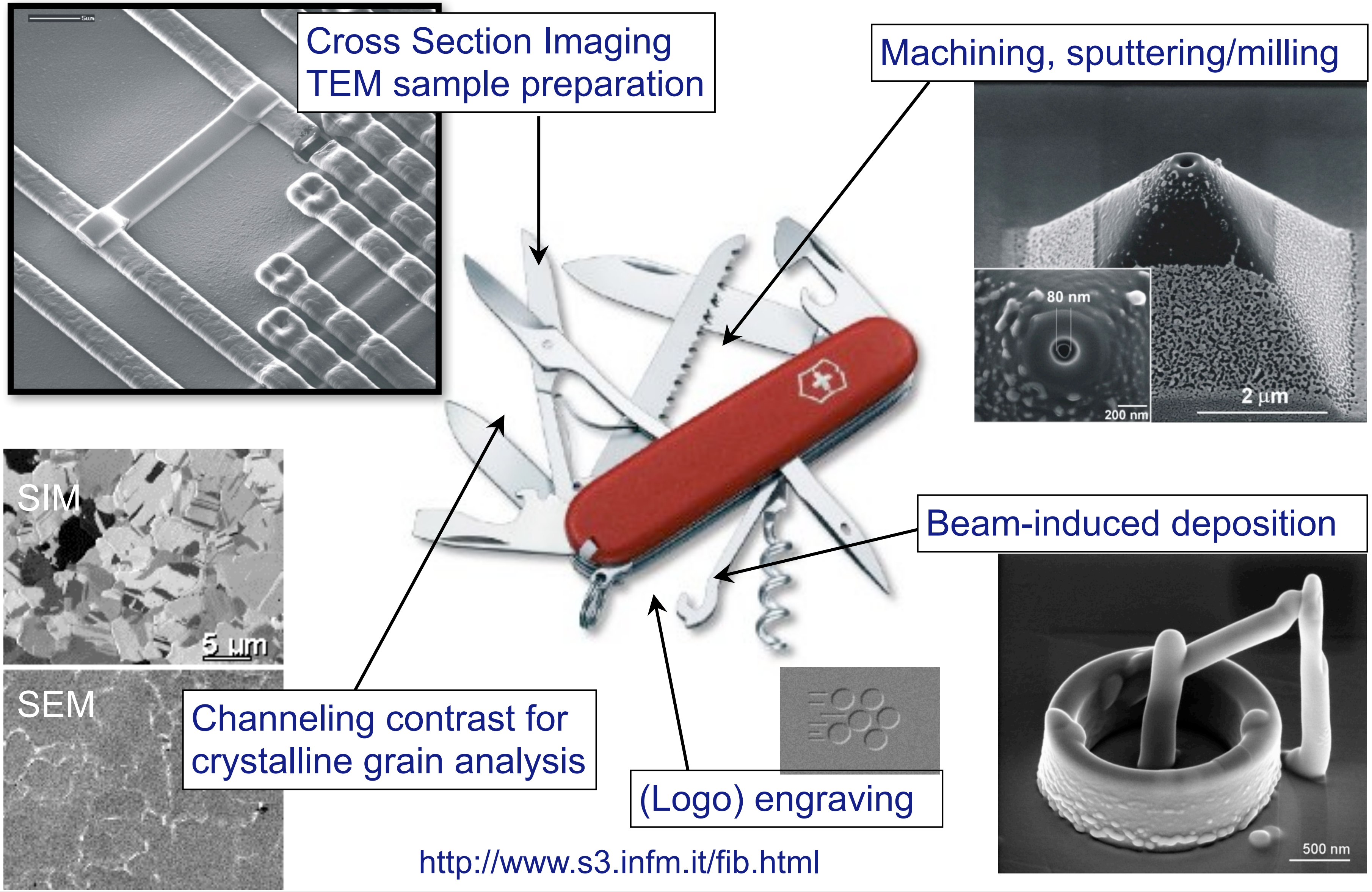
Killian et al.,
PRL **83**, 4776 (1999)

Ultracold Electron/Ion Source



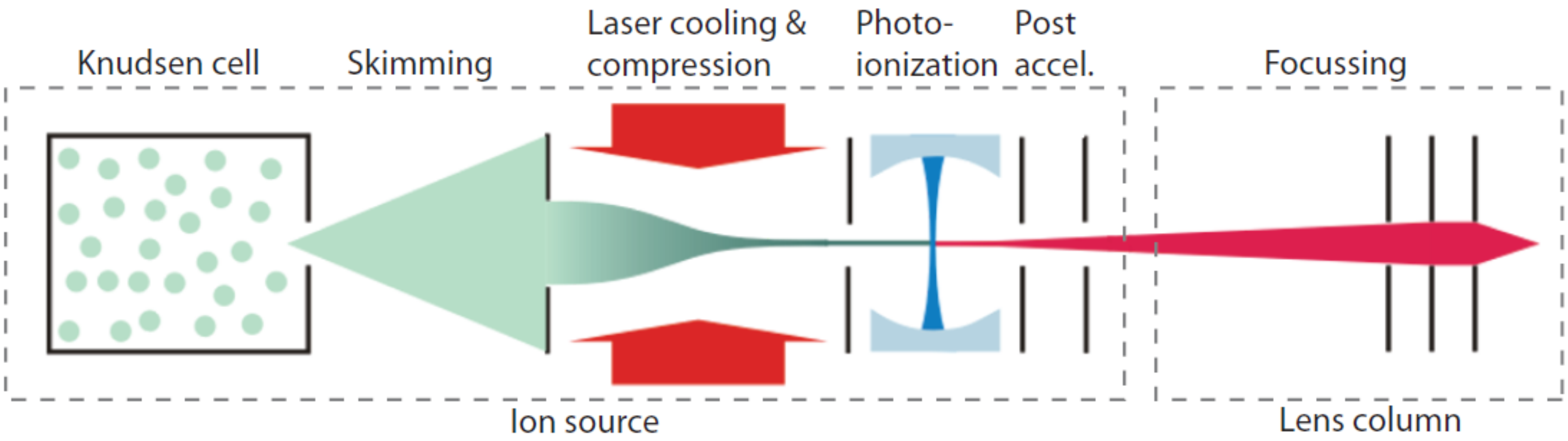
Trap & Cool	**Ionize**	**Accelerate**
Magneto-optical trap	**Ultracold plasma**	**Ultracold source**
Density ≈ 10^{16} / m^3 RMS size ≈ 1 mm T = 100 μK	Ionization radius ≈ 50 μm	Bunch energy E = 15 keV
	Killian et al., PRL **83**, 4776 (1999)	Luiten et al., PRL **95**, 164801 (2005) McCulloch et al., Nat. Phys. **7**, 785 (2011)

Application: Focused ion beams (FIB)



Application: Focused ion beam

- **Aim: Lots of current at nm spotsizes**
- Design disaster: Beams heats up during acceleration



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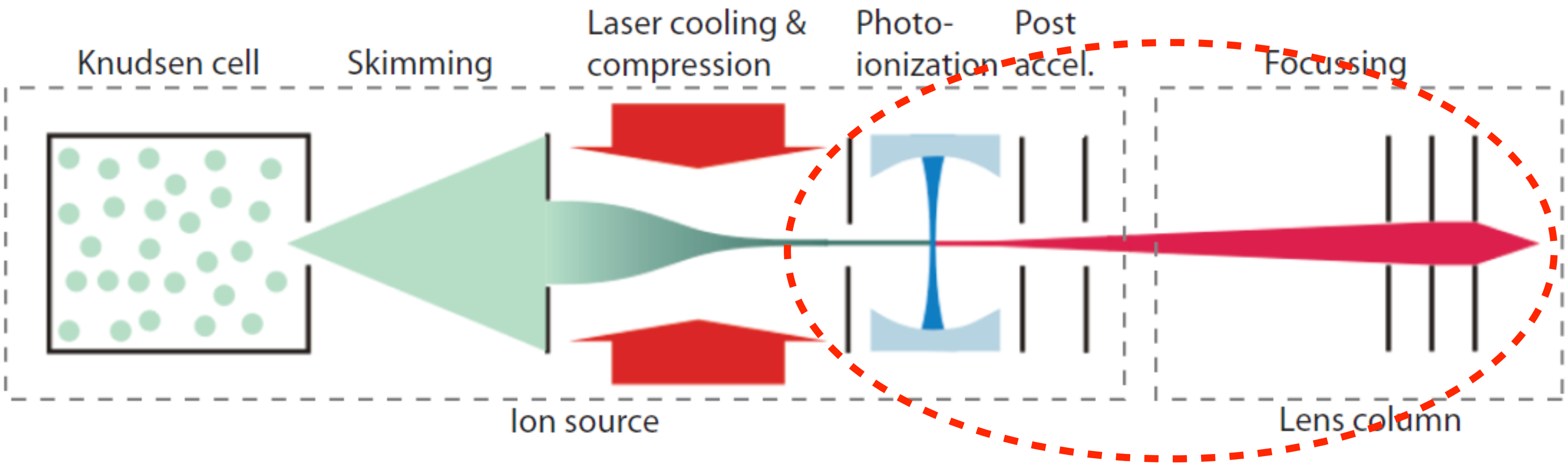


‘Typical’ simulation code: GPT

www.pulsar.nl

Tracks sample particles in **time-domain**

- Relativistic equations of motion
- Fully 3D, including all non-linear effects

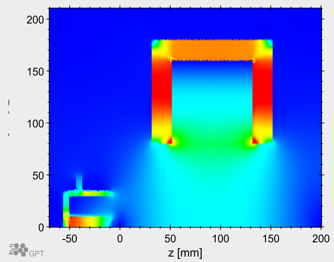
- GPT solves with 5[th] order embedded Runge Kutta, adaptive stepsize
- GPT 3.2 beta includes a multi-objective genetic optimizer
- Challenge: **E**(**r**,t), **B**(**r**,t), flexibility without compromising accuracy

External fields

Analytical expressions

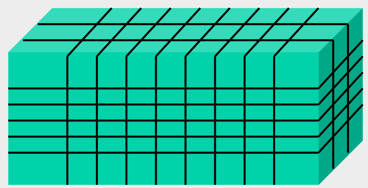
$\{E,B\}=f(x,y,z,t)$

Field-maps

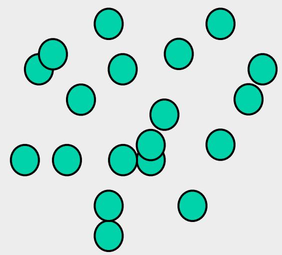


Coulomb interactions

Particle in Cell



All interactions



www.pulsar.nl

Coulomb interactions

Macroscopic (mean field):

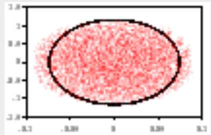
- **Space-charge**
- Average repulsion force
- Bunch expands
- Deformations in phase-space
- Governed by Poisson’s equation

Microscopic:

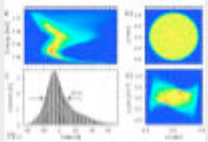
- **Disorder induced heating**
- Neighbouring particles ‘see’ each other
- Potential energy → momentum spread
- Stochastic effect
- Governed by point-to-point interactions

GPT simulations

PRL *93, 094802*
O.J. Luiten et. al.

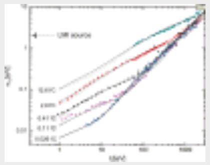


JAP 102, 093501
T. van Oudheusden et. al.

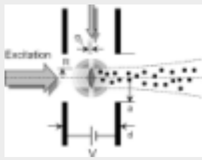


PRST-AB *9, 044203*
S.B. van der Geer et. al.

PRL *102, 034802*
M. P. Reijnders et. al.

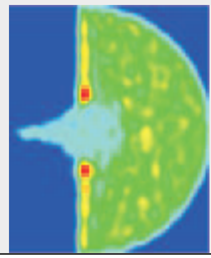


JAP *102, 094312*
S.B. van der Geer et. al.



Nature *Photonics*
Vol 2, May 2008
M. Centurion et. al.

And many others…

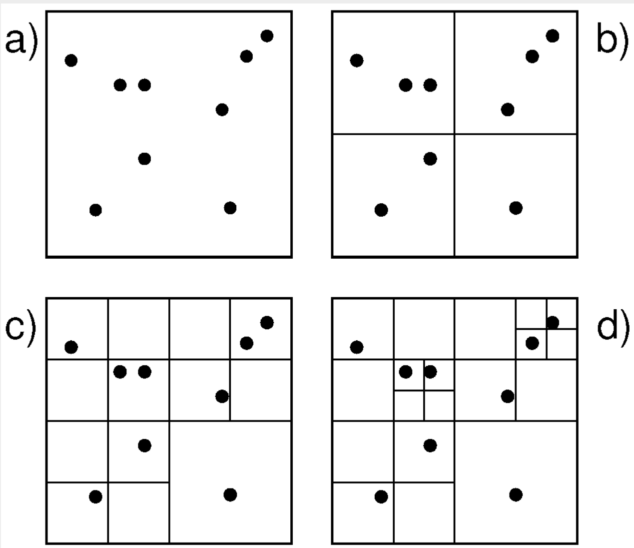


Barnes-Hut

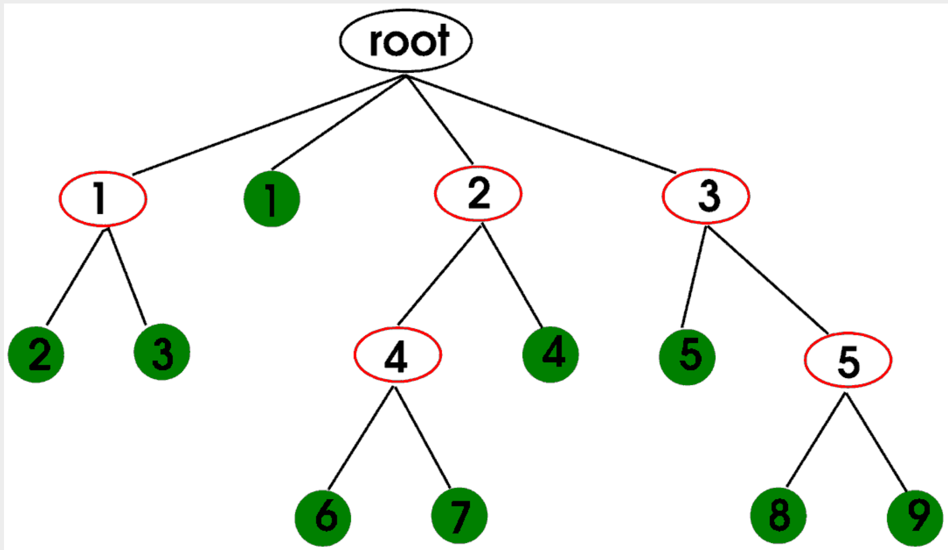
Hierarchical tree algorithm:

- Includes *all* Coulomb interactions
- O(N log N) in CPU time
- User-selectable accuracy

Division of space



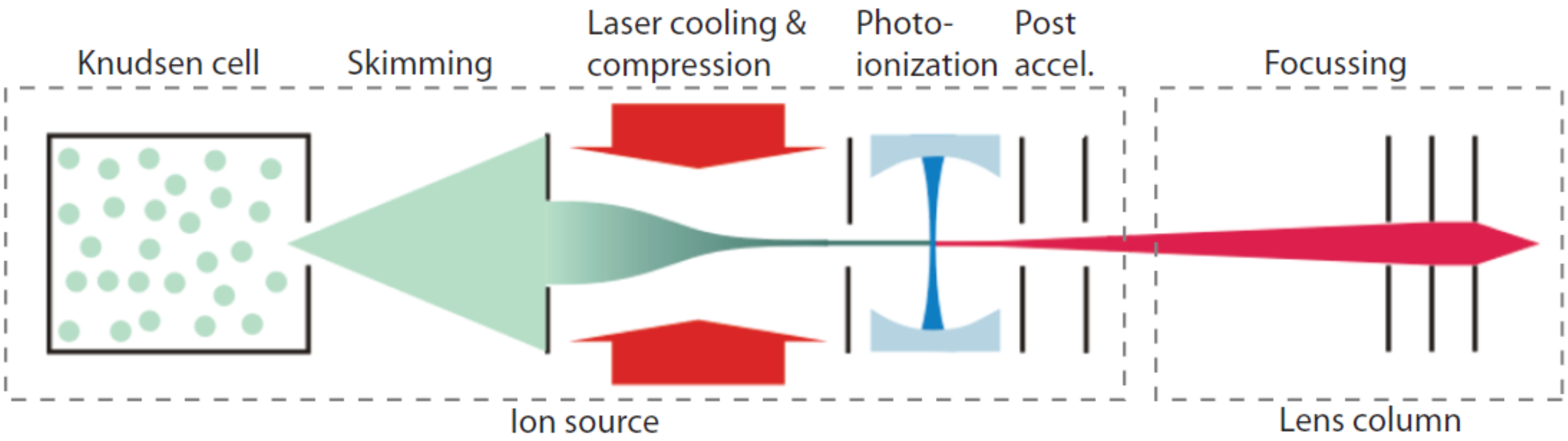
Tree data structure



J. Barnes and P. Hut, Nature **324**, (1986) p. 446.

Application: Focused ion beam

- **Aim: Lots of current at nm spotsizes**
- Design disaster: Beams heats up during acceleration
- **Multi-objective global optimization**



Kalyanmoy Deb et. al., A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II, IEEE Transactions On Evolutionary Computation, Vol. 6, No. 2, A

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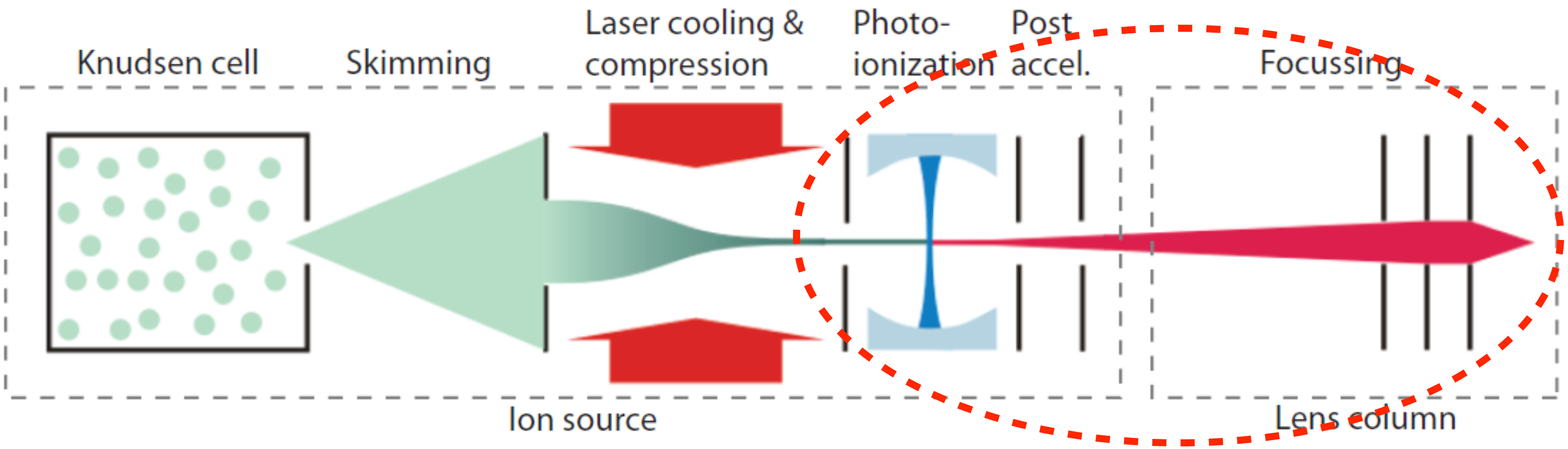

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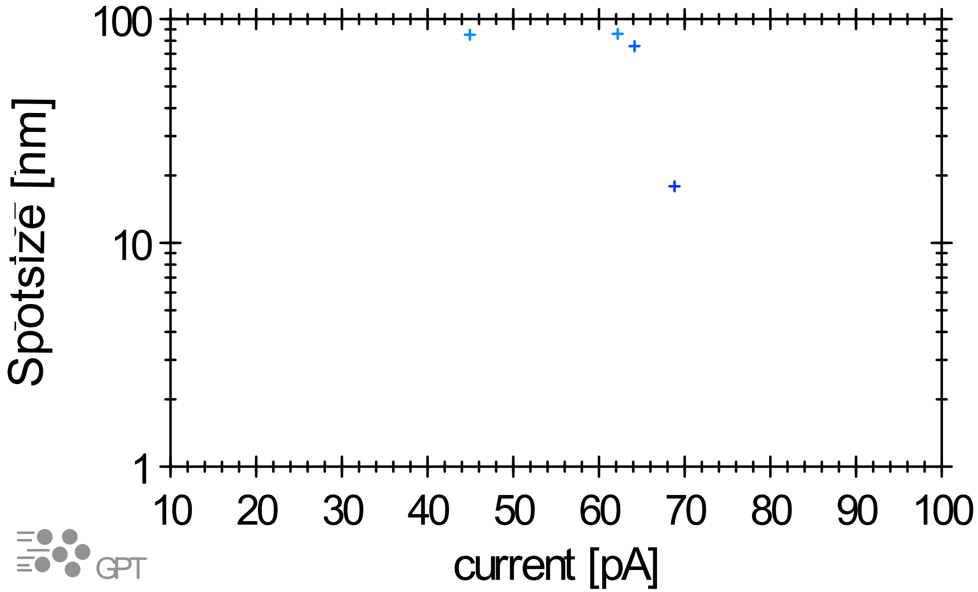
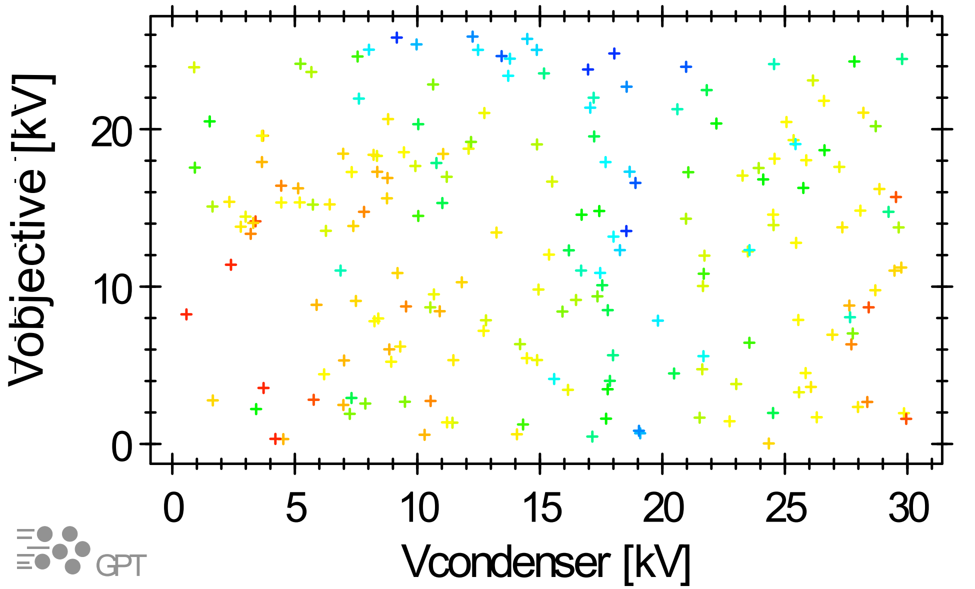
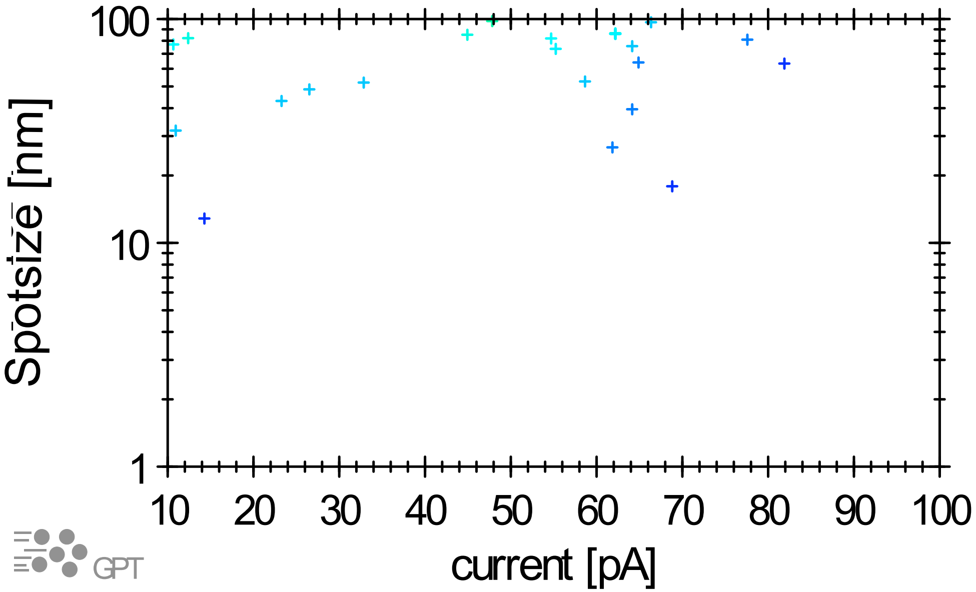


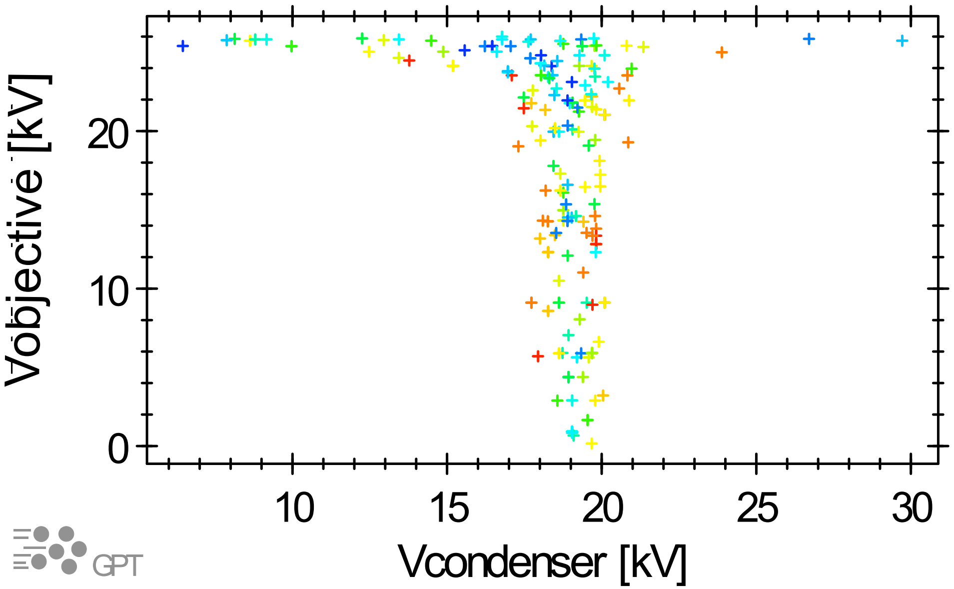


Initial population:

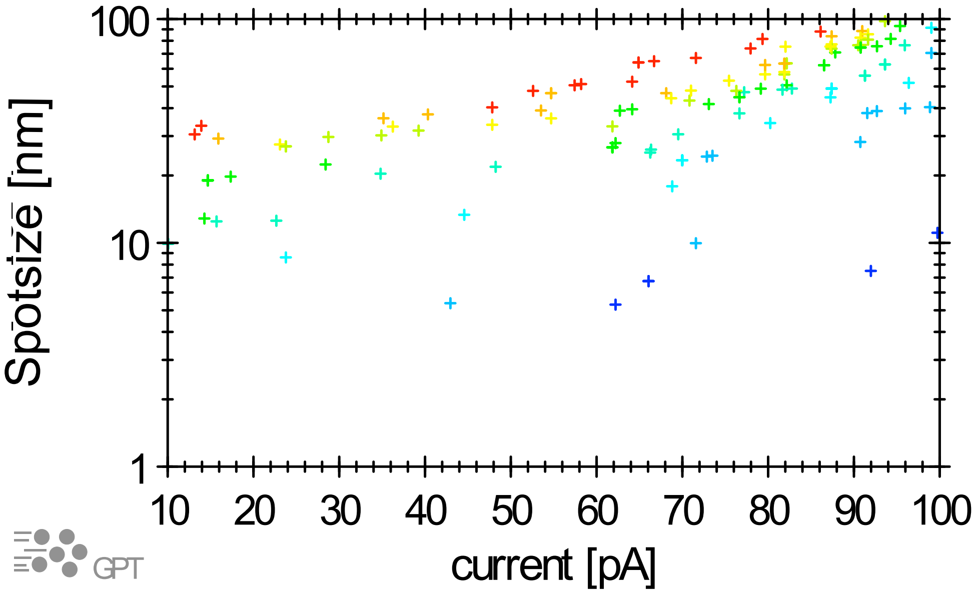
Very large spotsizes

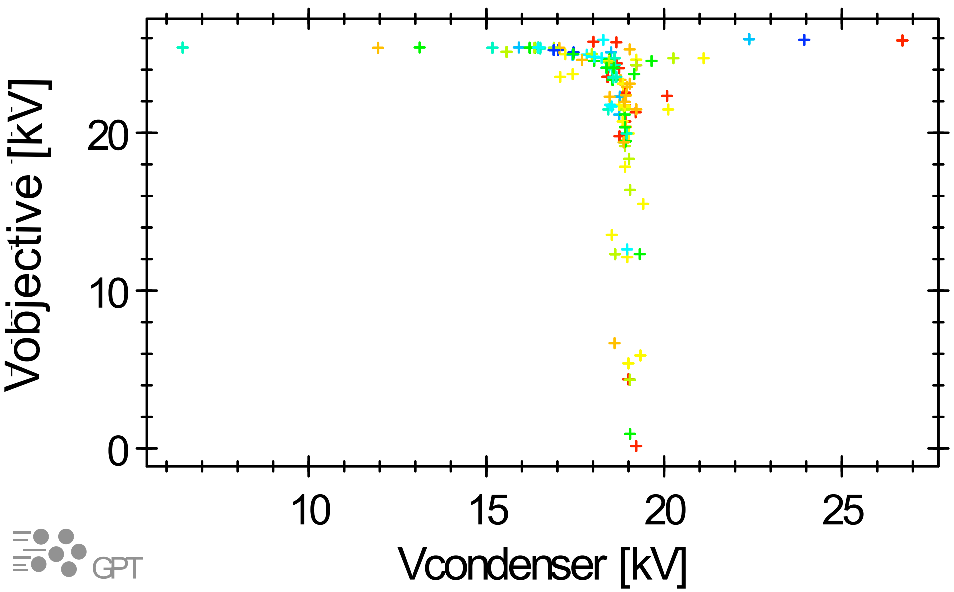
Off scale

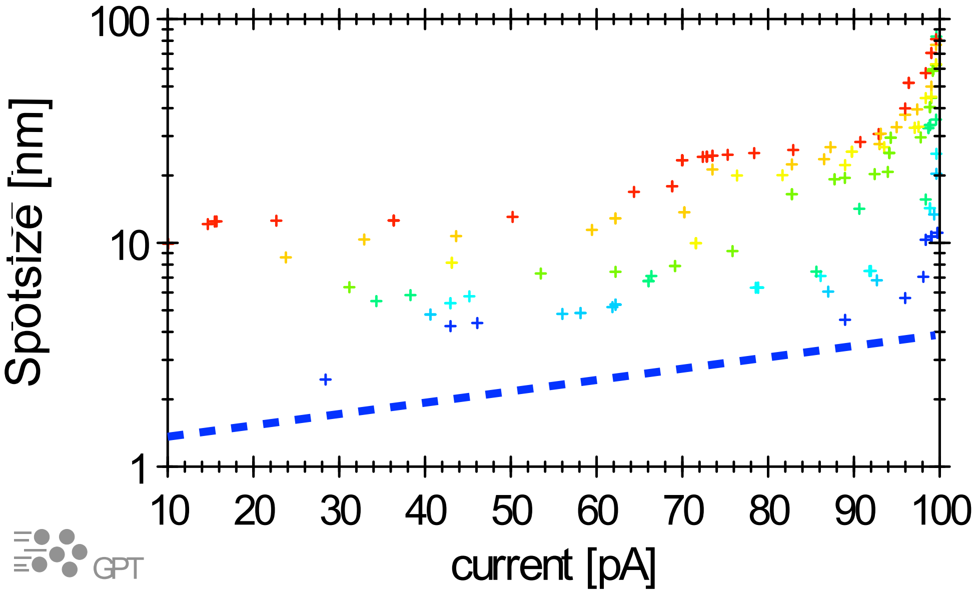




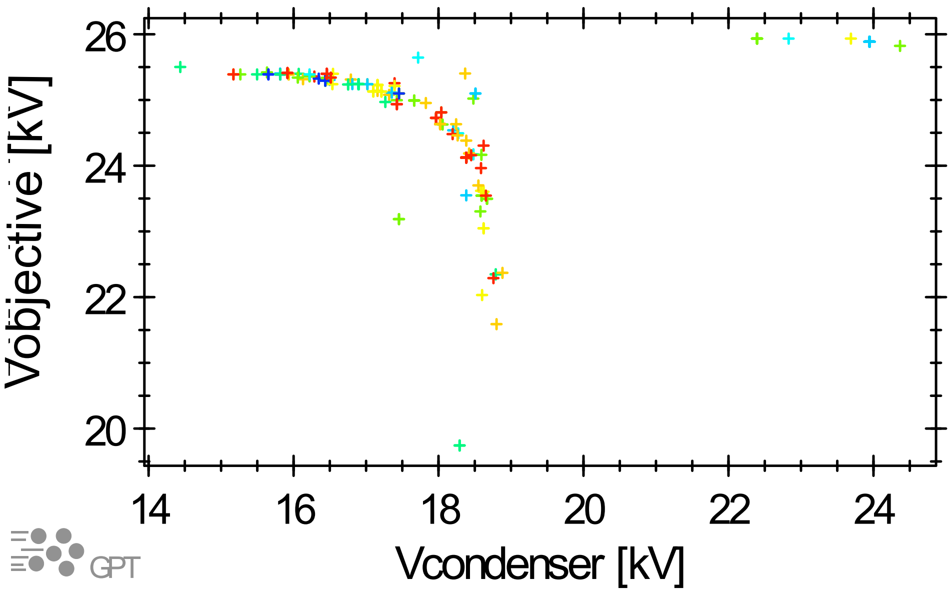
Initial steps:
Volume in variable space significantly reduced

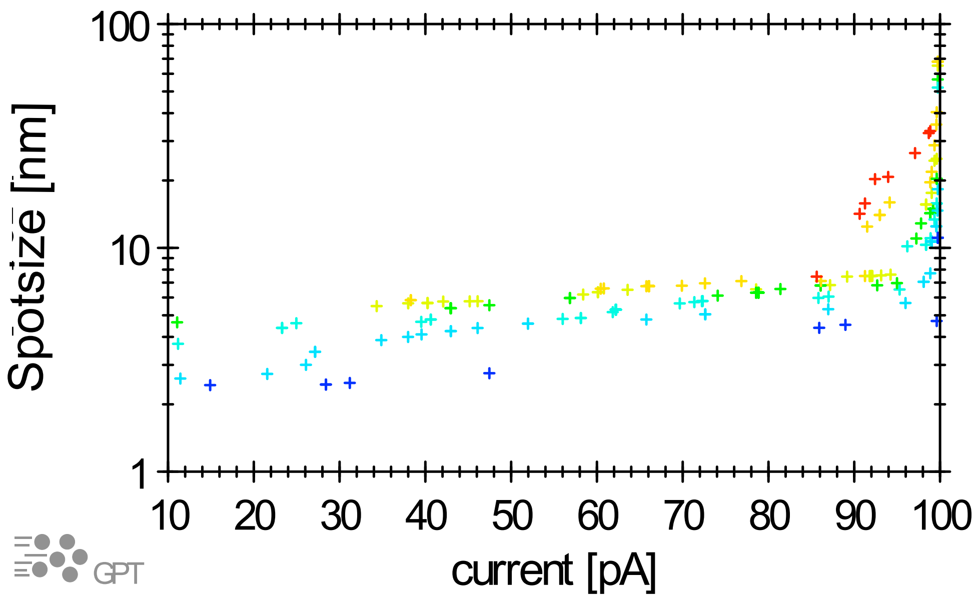

100
10
1
Spotsize [nm]
10
20
30
40
50
60
70
80
90
100
current [pA]
GPT

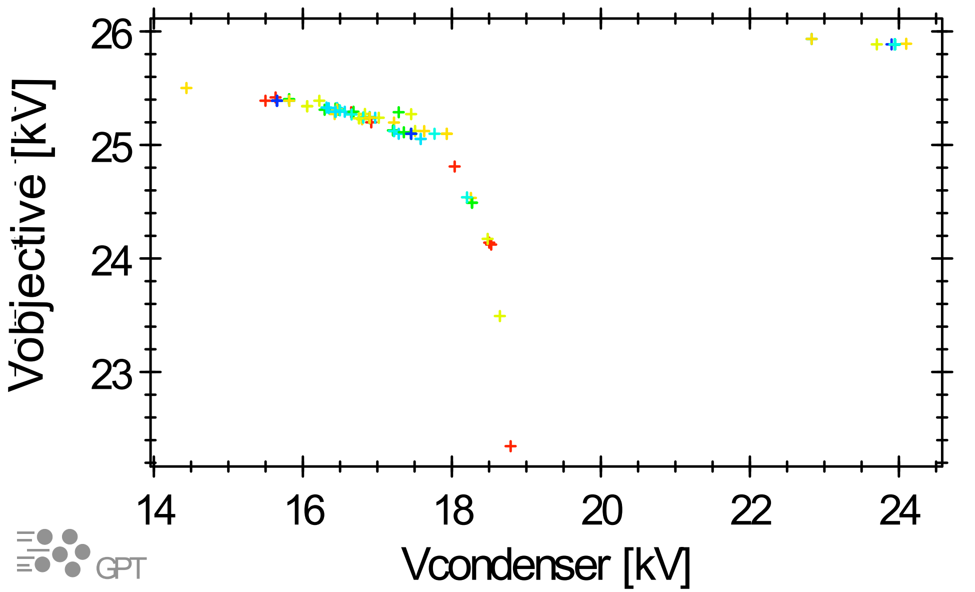

20
10
0
Vobjective [kV]
10
15
20
25
Vcondenser [kV]
GPT

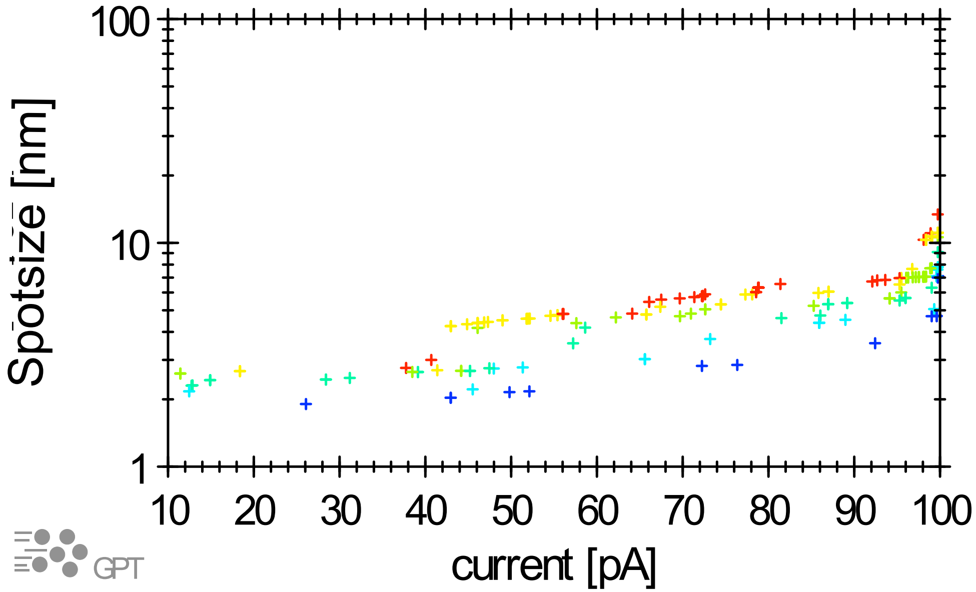


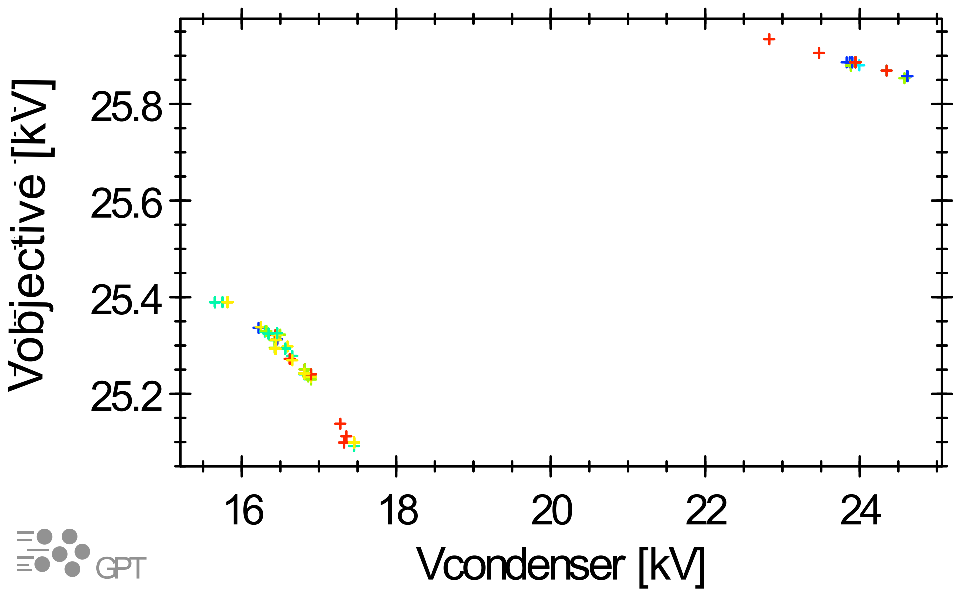
Pareto front:
Impossible to improve one objective without degrading at least one other objective




100
10
1
10 20 30 40 50 60 70 80 90 100
current [pA]
Spotsize [nm]
GPT


26
25
24
23
14 16 18 20 22 24
Vcondenser [kV]
Vobjective [kV]
GPT





Break-up in variable space:

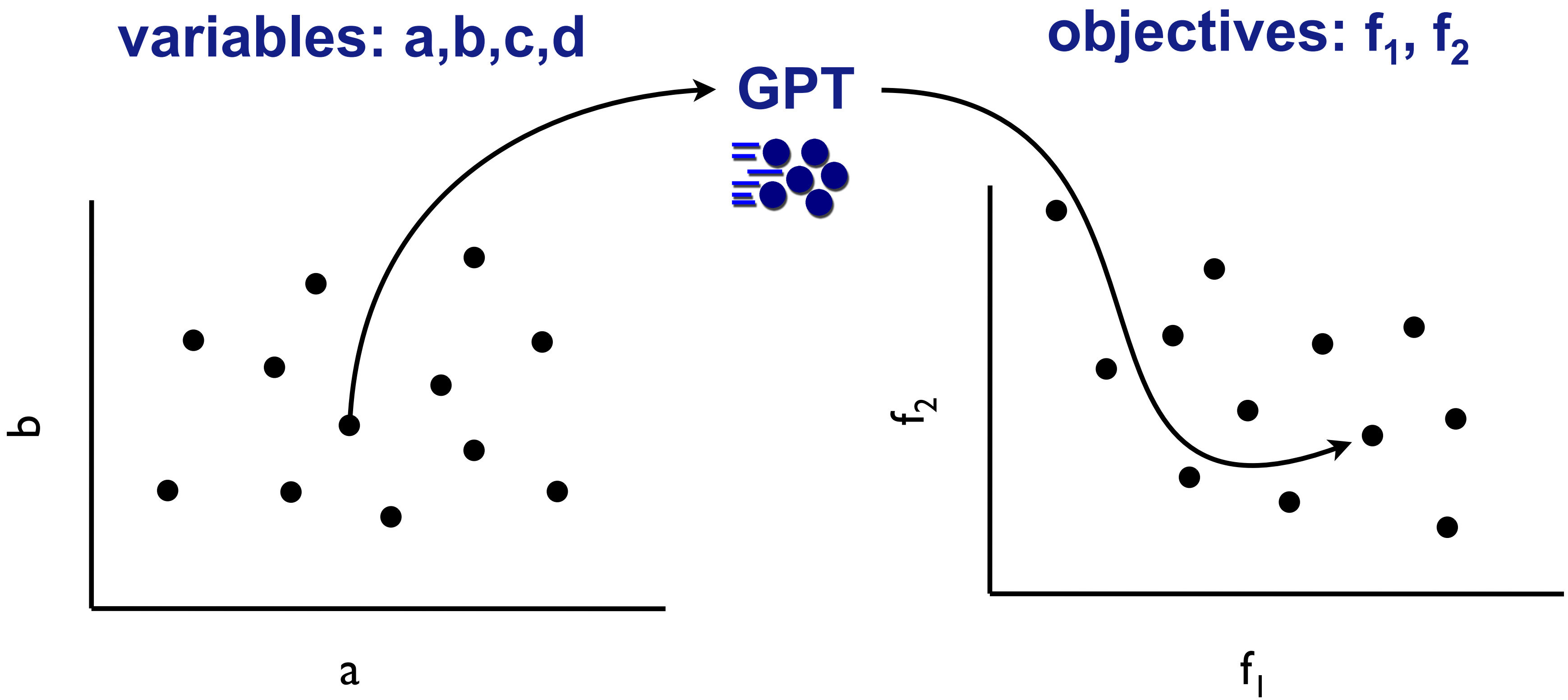
Different scenario's:

With and without crossover

4 slides are intentionally removed

Variables and objectives

- **Objectives f_n are a function of all variables**
  - **$f_1(a,b,c,d)$, $f_2(a,b,c,d)$, ...**



The problem: Too many knobs to turn

The solution: Multi-objective optimization

Multi-objective optimization

- **Work iteratively with a population of samples**

- **At each iteration:**
  - **Add new samples using ‘best’ samples in population**
  - **Remove “worst’ samples**

- **Aim:**
  - **Nicely sampled pareto front**

PHYSICAL REVIEW SPECIAL TOPICS - ACCELERATORS AND BEAMS **14**, 072001 (2011)

Comparison of dc and superconducting rf photoemission guns for high brightness high average current beam production

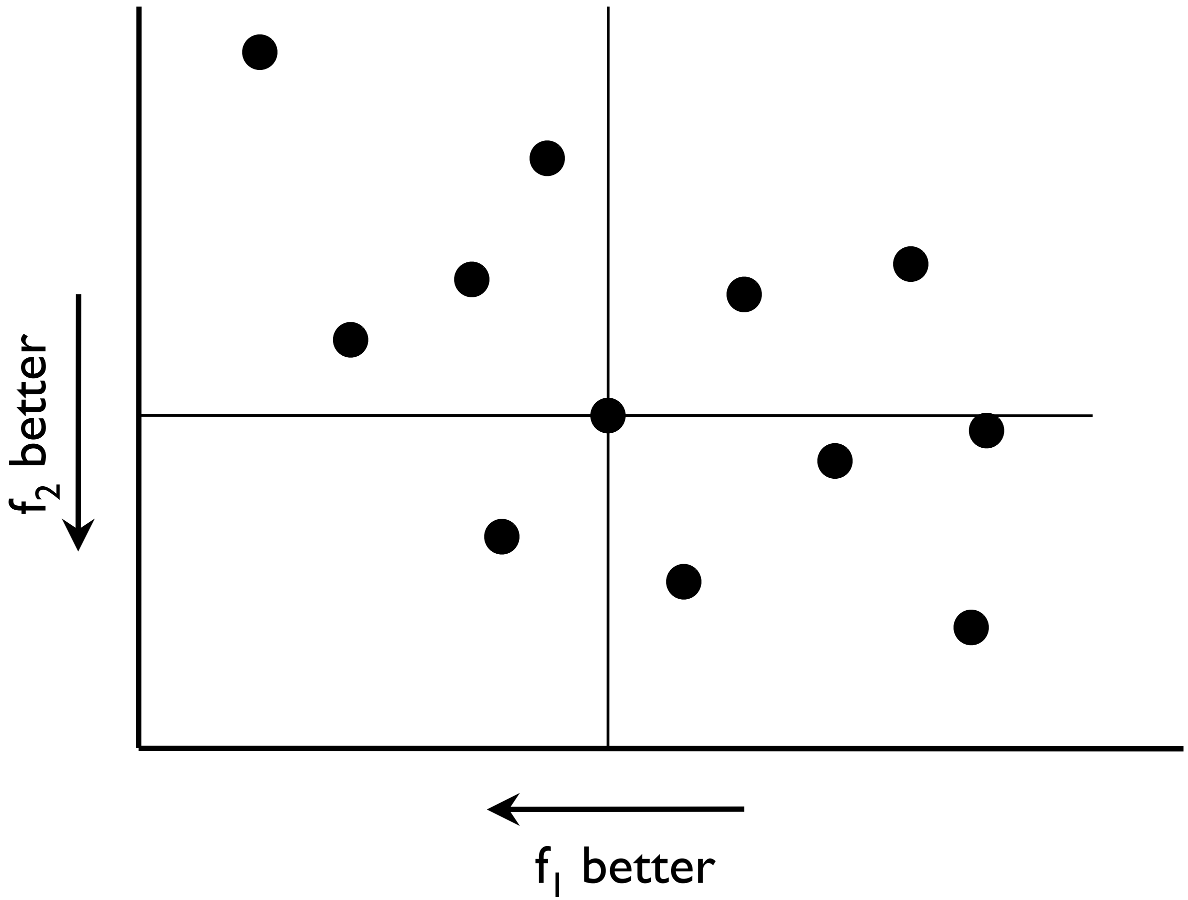
Ivan V. Bazarov, Allen Kim, Manu N. Lakshmanan, and Jared M. Maxson
Cornell Laboratory for Accelerator-based Sciences and Education, Cornell University, Ithaca, New York 14853, USA

TUAAI2 Proceedings of ICAP2012, Rostock-Warnemünde, Germany

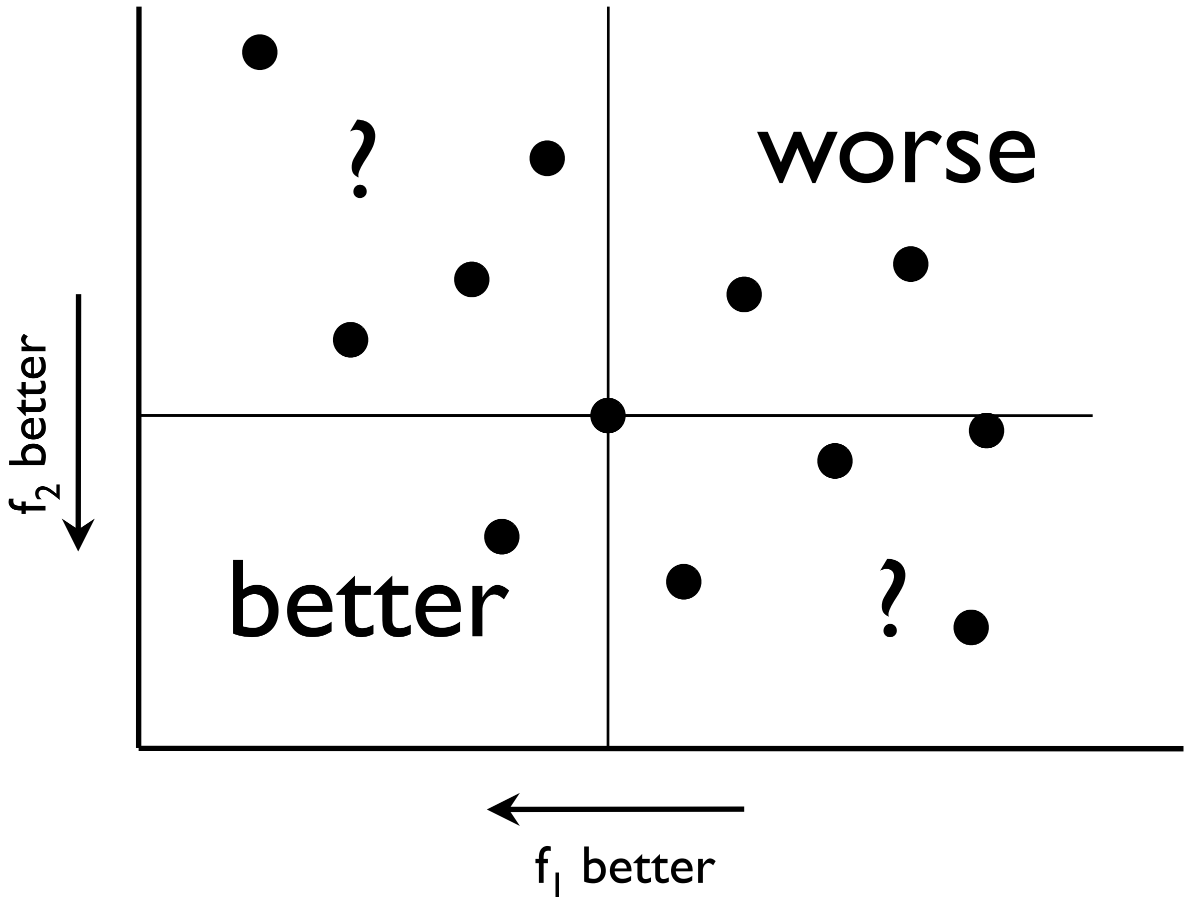
A MASSIVELY PARALLEL GENERAL PURPOSE MULTI-OBJECTIVE OPTIMIZATION FRAMEWORK, APPLIED TO BEAM DYNAMIC STUDIES

Y. Ineichen, A. Adelmann*, PSI, Villigen, Switzerland
C. Bekas, A. Curioni, IBM Research – Zurich, Switzerland
P. Arbenz, Department of Computer Science, ETH Zurich, Switzerland

Domination

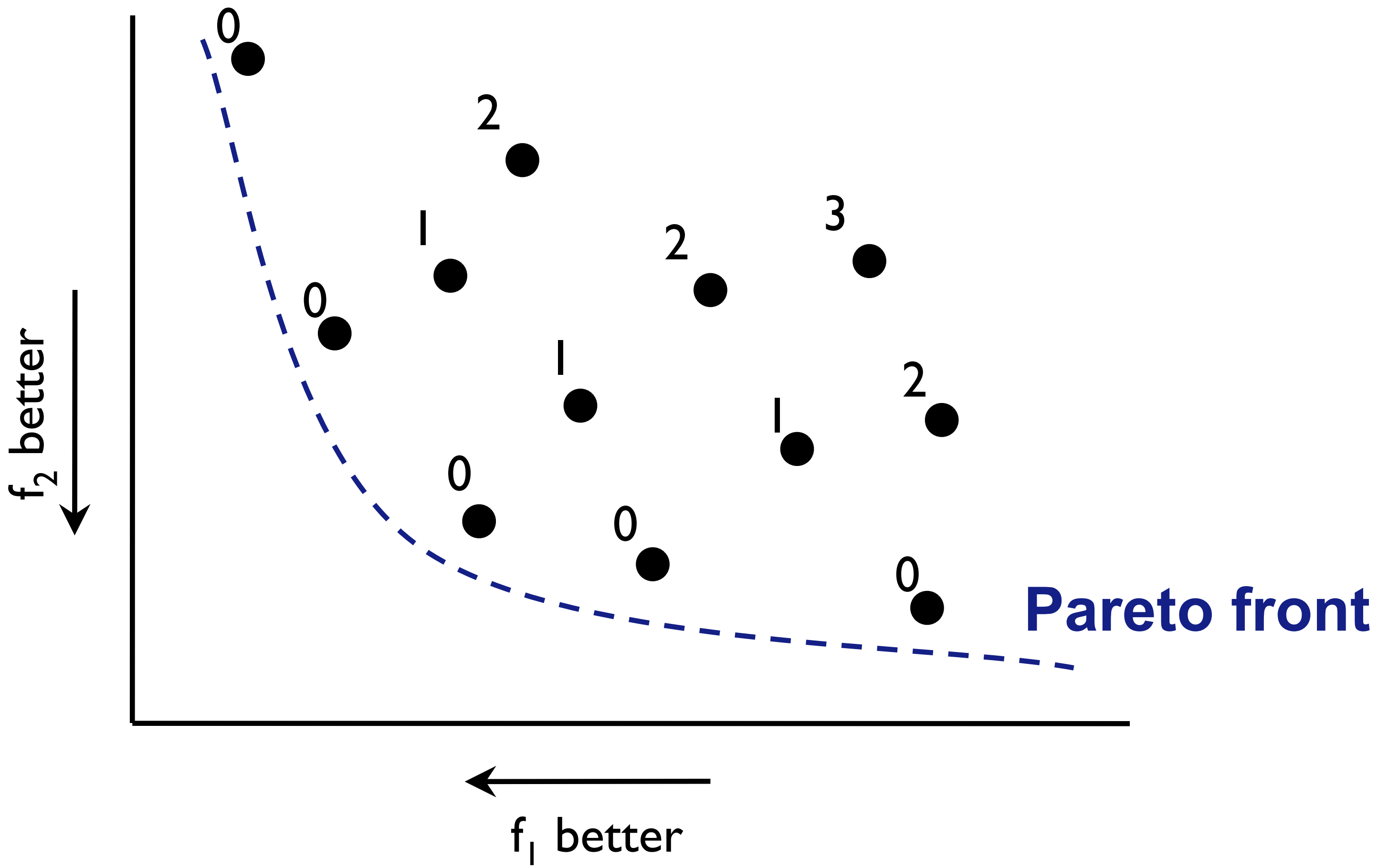


Domination: Who dominates who



Algorithm: Rank on domination and remove

- **Ranking starts closest to (unknown) pareto front**



A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II, Kalyanmoy Deb et al,
IEEE TRANSACTIONS ON EVOLUTIONARY COMPUTATION, VOL. 6, NO. 2, APRIL 2002

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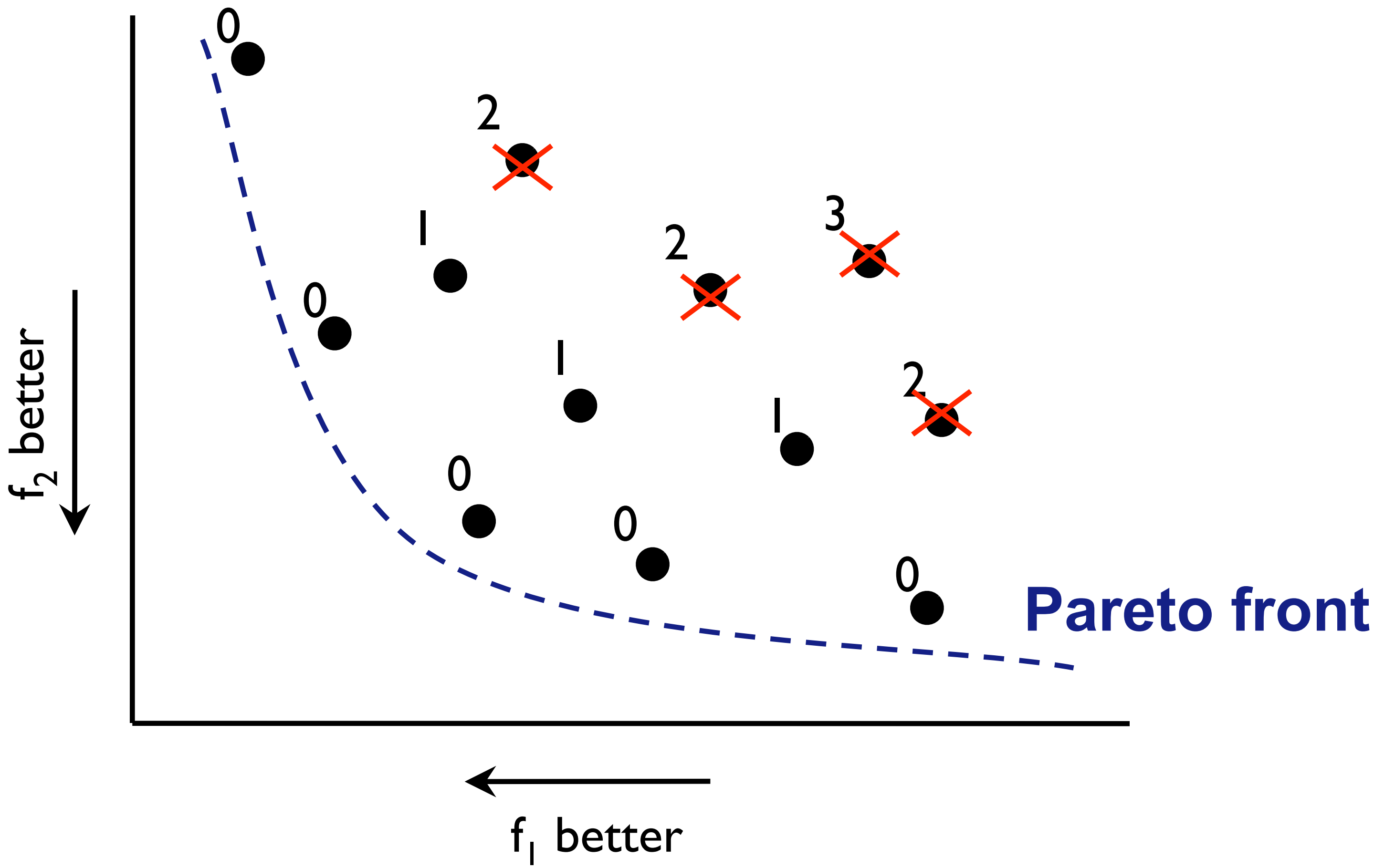
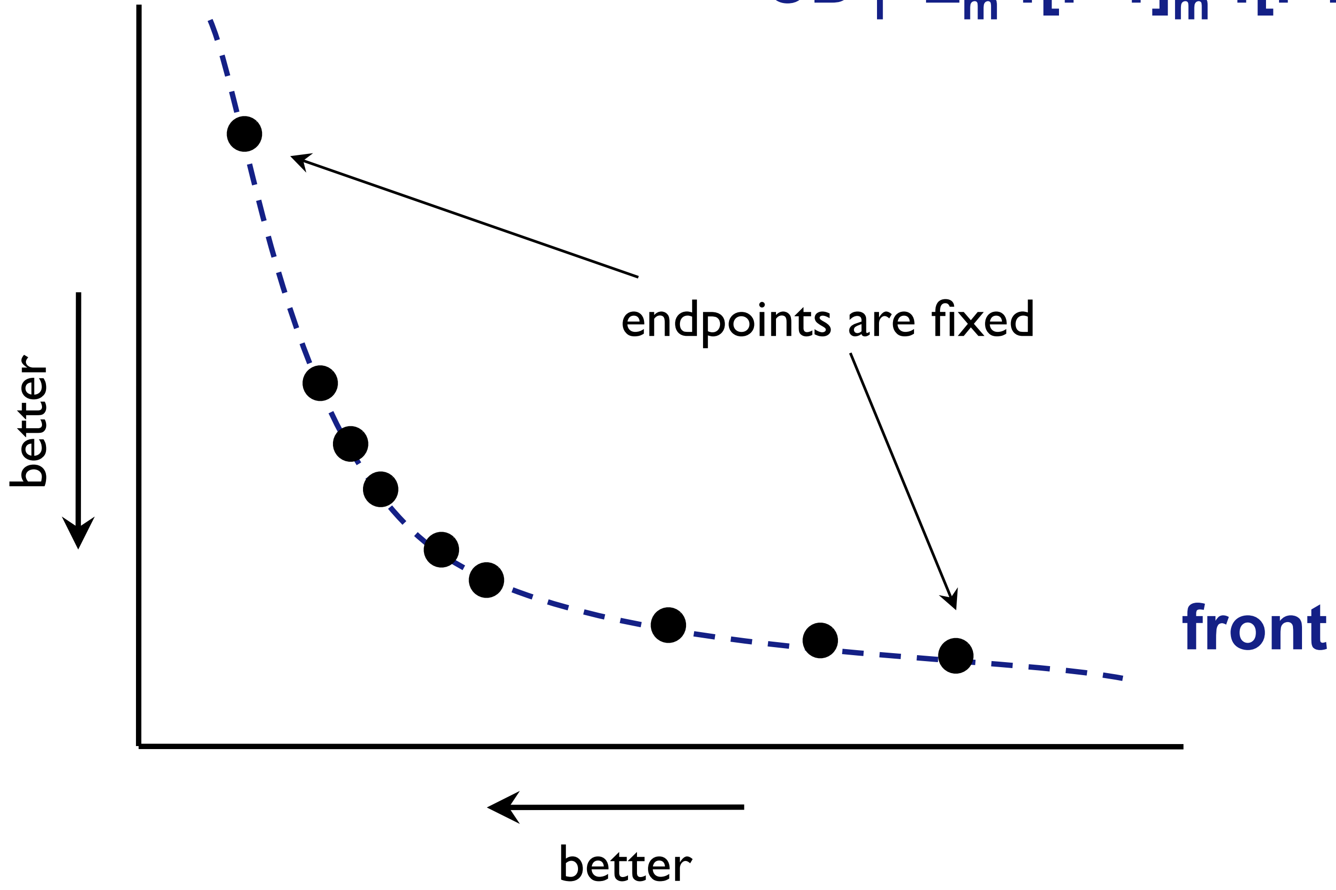


A Fast and Elitist Multiobjective Genetic Algorithm: NSGA-II, Kalyanmoy Deb et al,
IEEE TRANSACTIONS ON EVOLUTIONARY COMPUTATION, VOL. 6, NO. 2, APRIL 2002

Algorithm: Uniform front

- **Crowding distance (CD)**
- **$CD_i = \Sigma_m f[i+1]_m - f[i-1]_m$**



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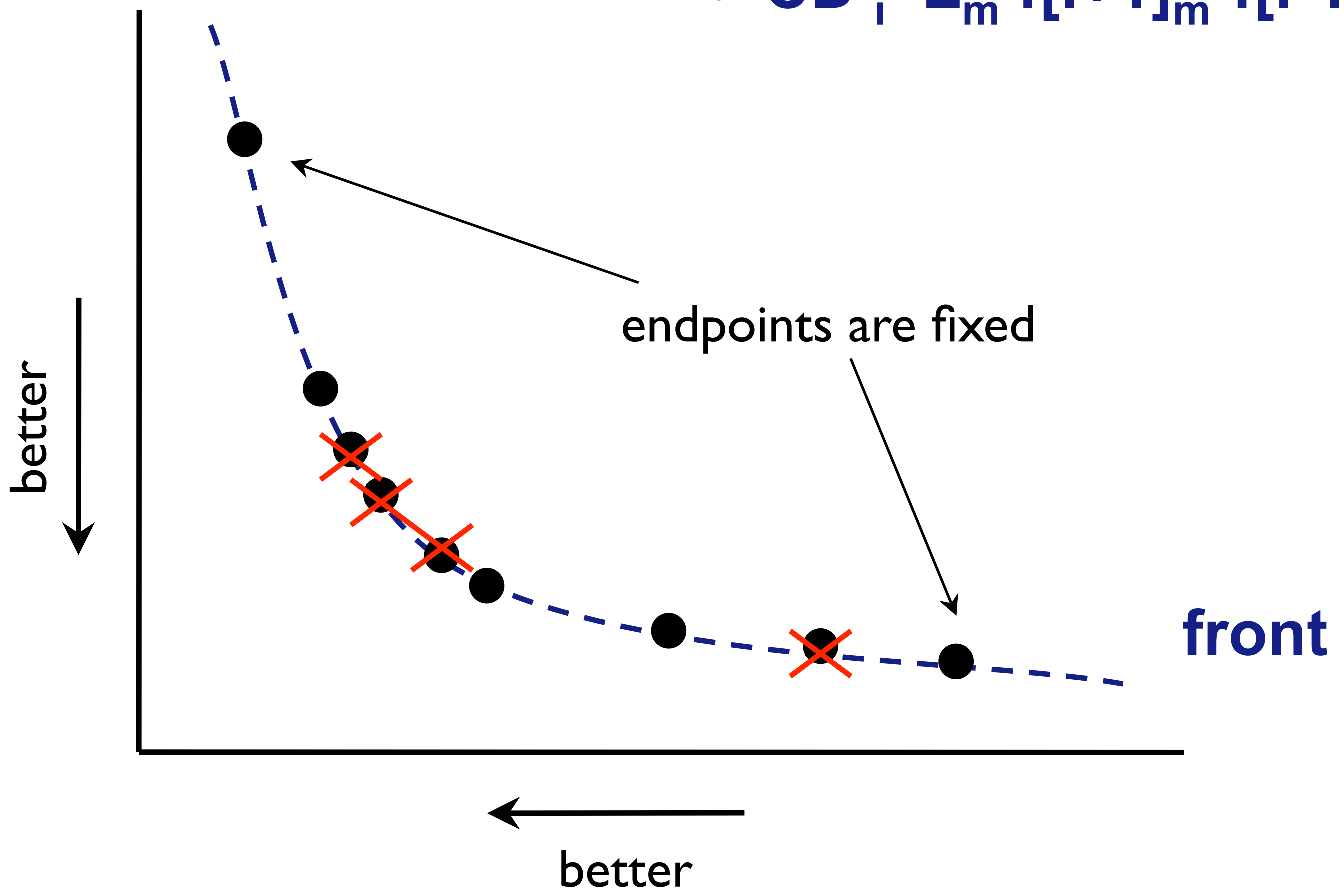
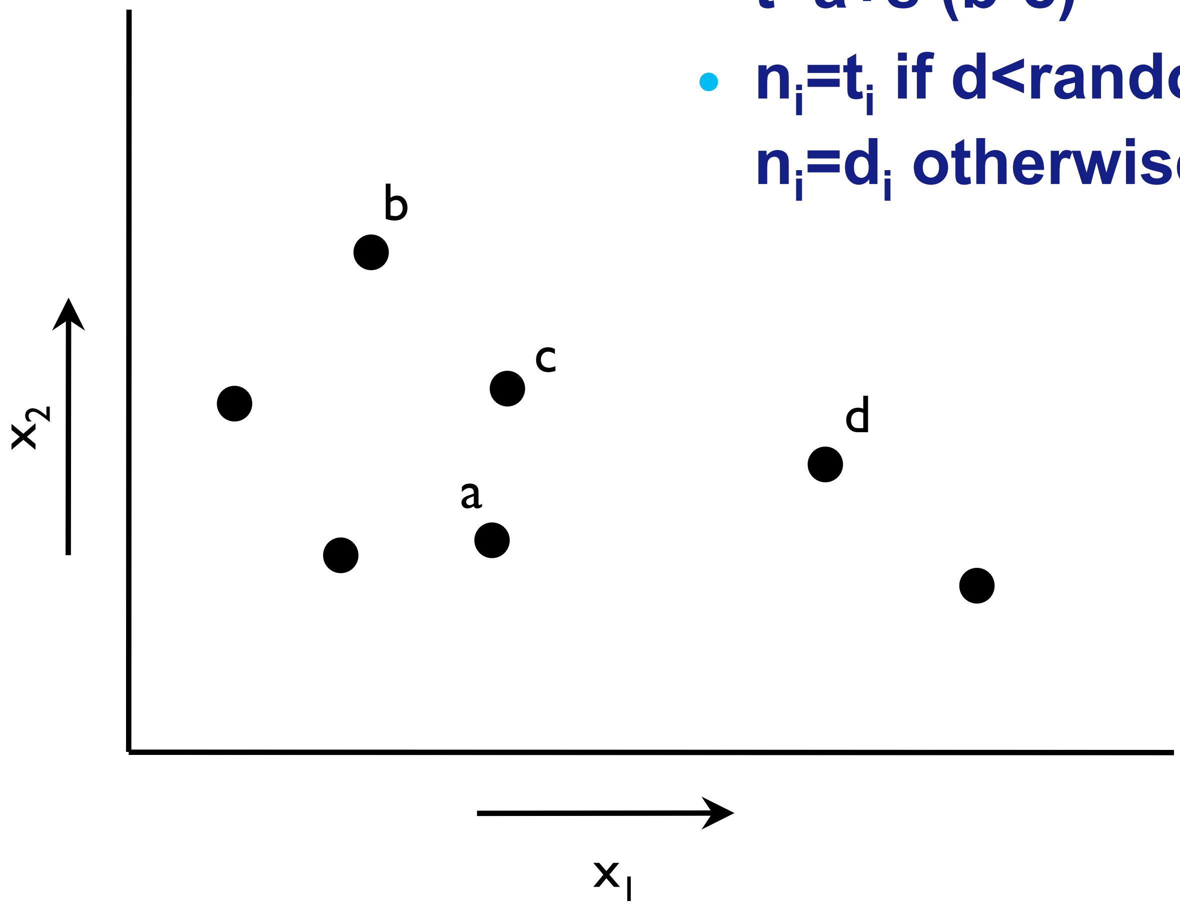


Algorithm: New points (just one method)

- Differential evolution

- Select 4 random points
- $t=a+s\ (b-c)$
- $n_i=t_i$ if $d<\text{random}(0,1)$
  $n_i=d_i$ otherwise



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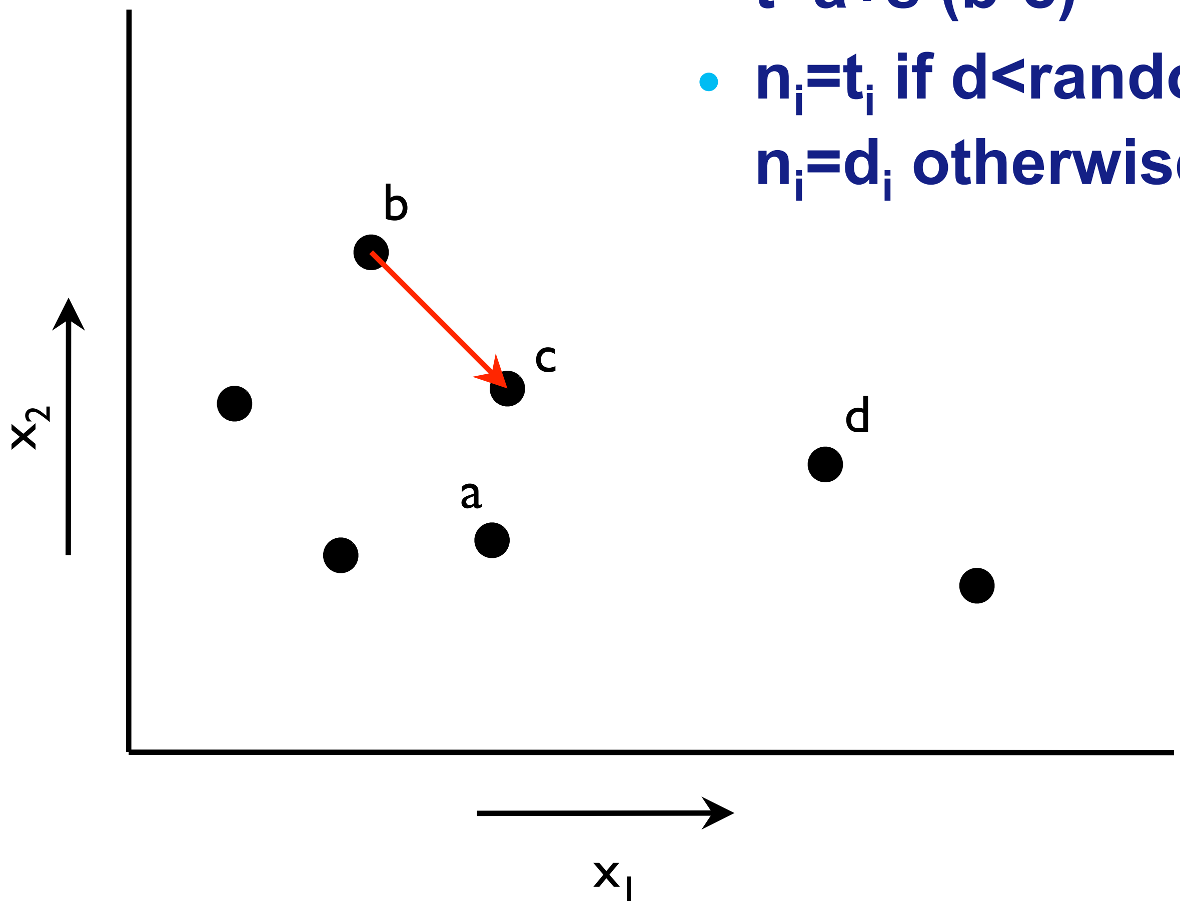

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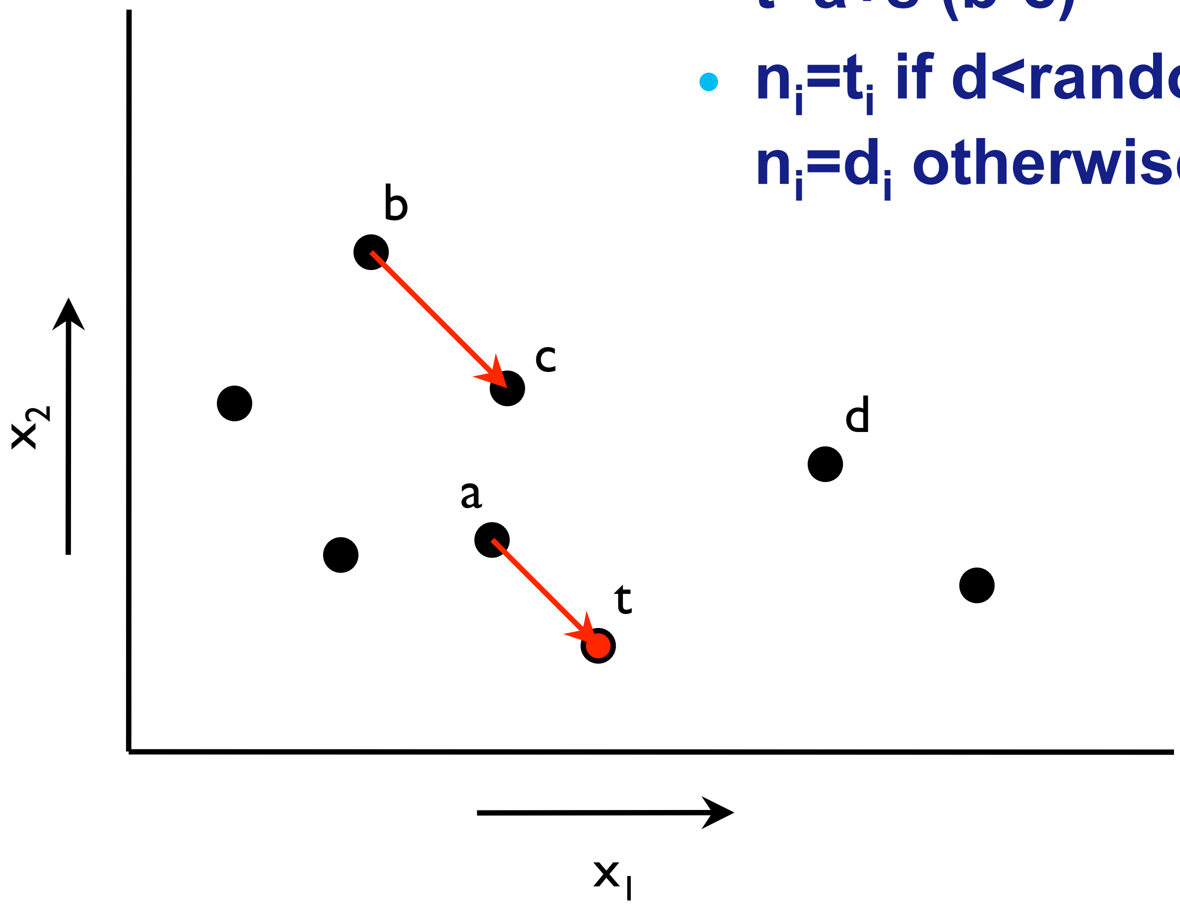

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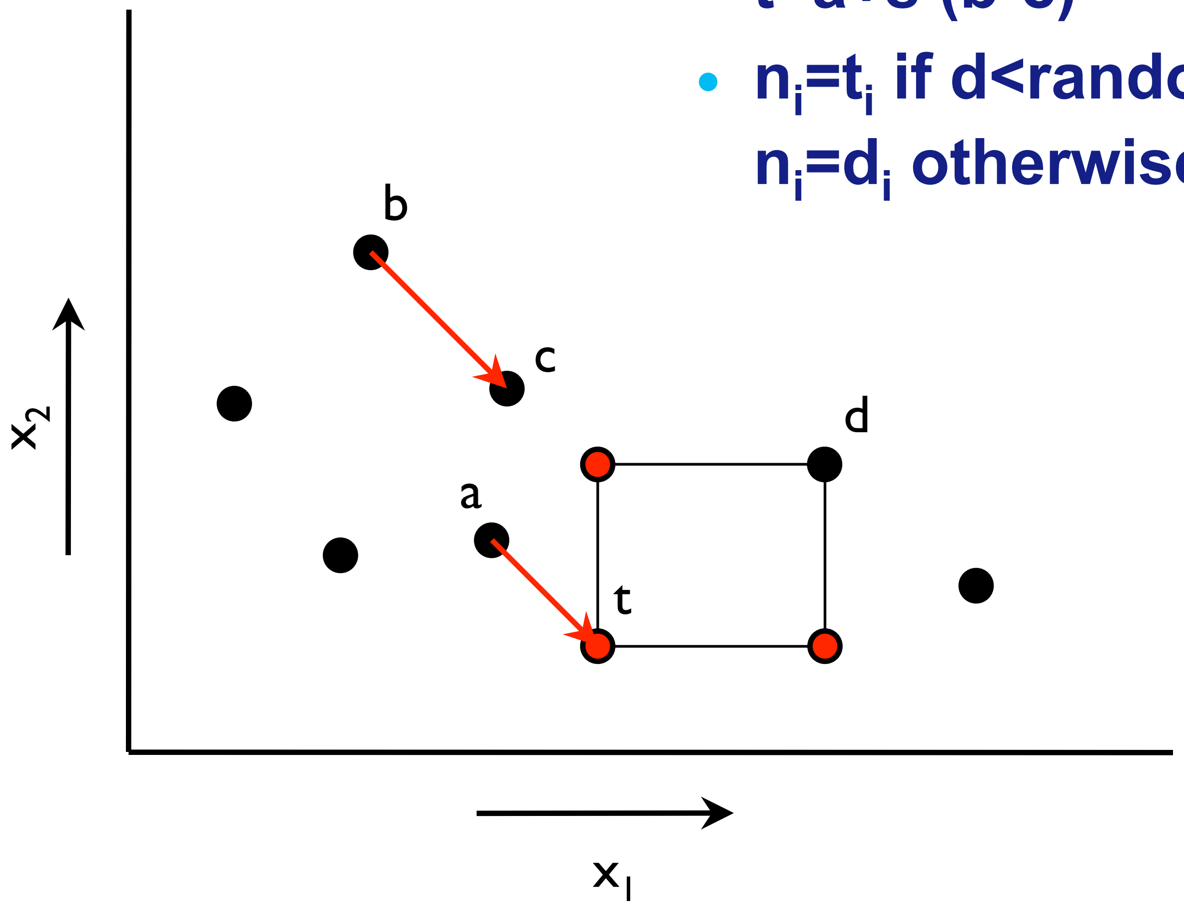


Algorithm: Constraints

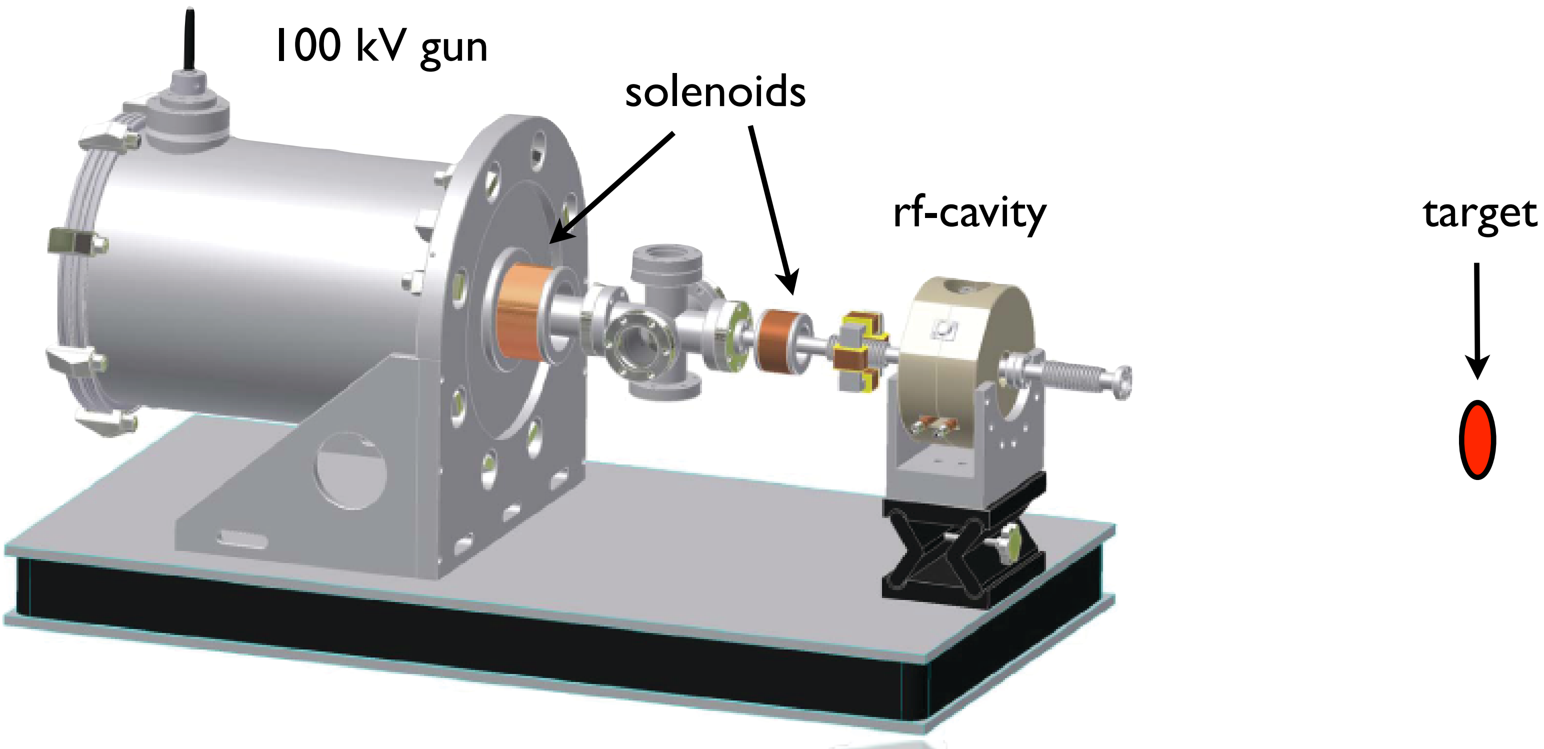
- In practice we always have
  - Multiple objectives
  - AND constraints

- Examples:
  - We need to stay within budget
    (but there is no point calculating the optimal design for each and every price)
  - We want a ‘short’ pulse at the target
    (but there is no point going below 100 fs since our detector has more jitter than that anyway)

- Constraints can easily be added to the sorting

Example: Utrafast electron diffraction

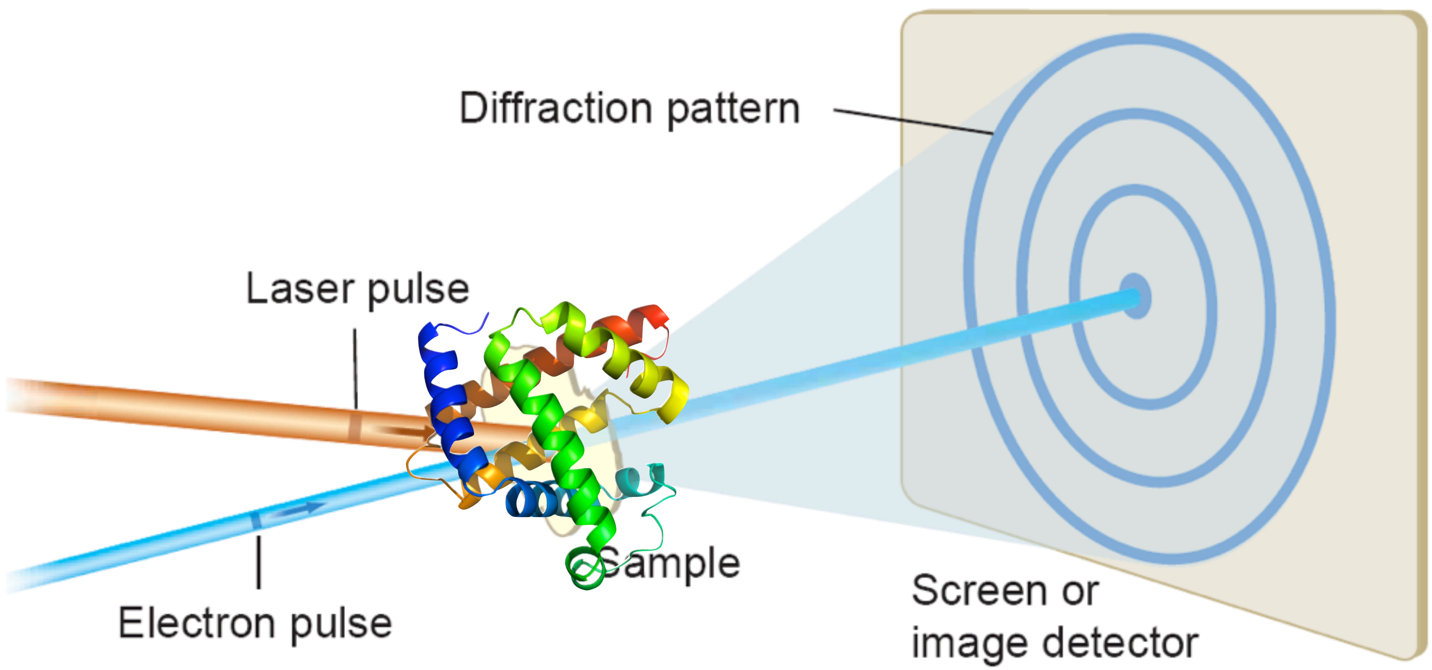
- **Variables: rf-amplitude, phase, solenoid1, solenoid2**
- **Conflicting objectives: Q, Lc, spot size, pulse length**
- **Performance dominated by non-linear effects**



T. van Oudheusden et. al., Physical Review Letters, 105 (26), art. no. 264801 (2010).

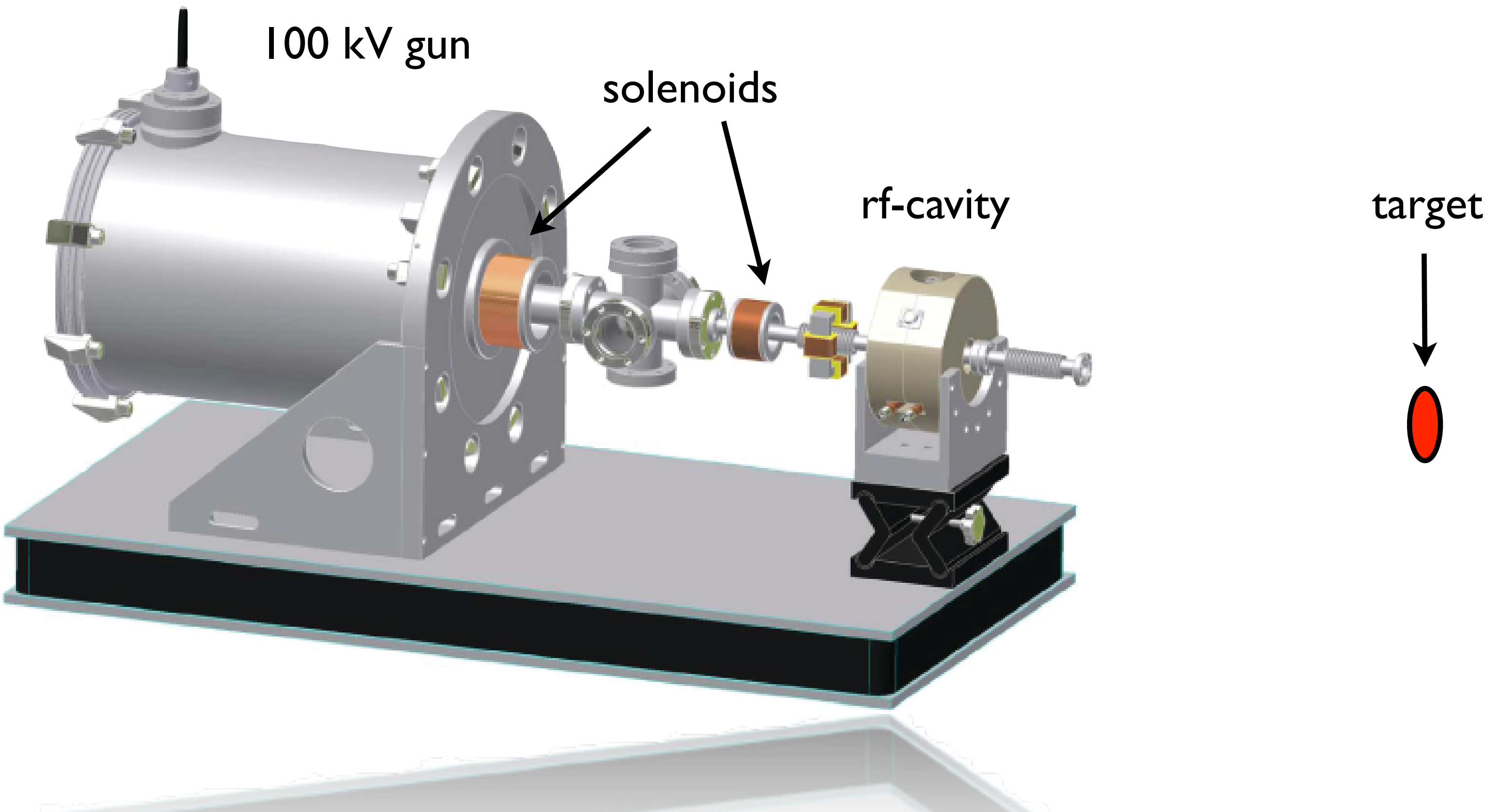
Application: Ultrafast electron diffraction

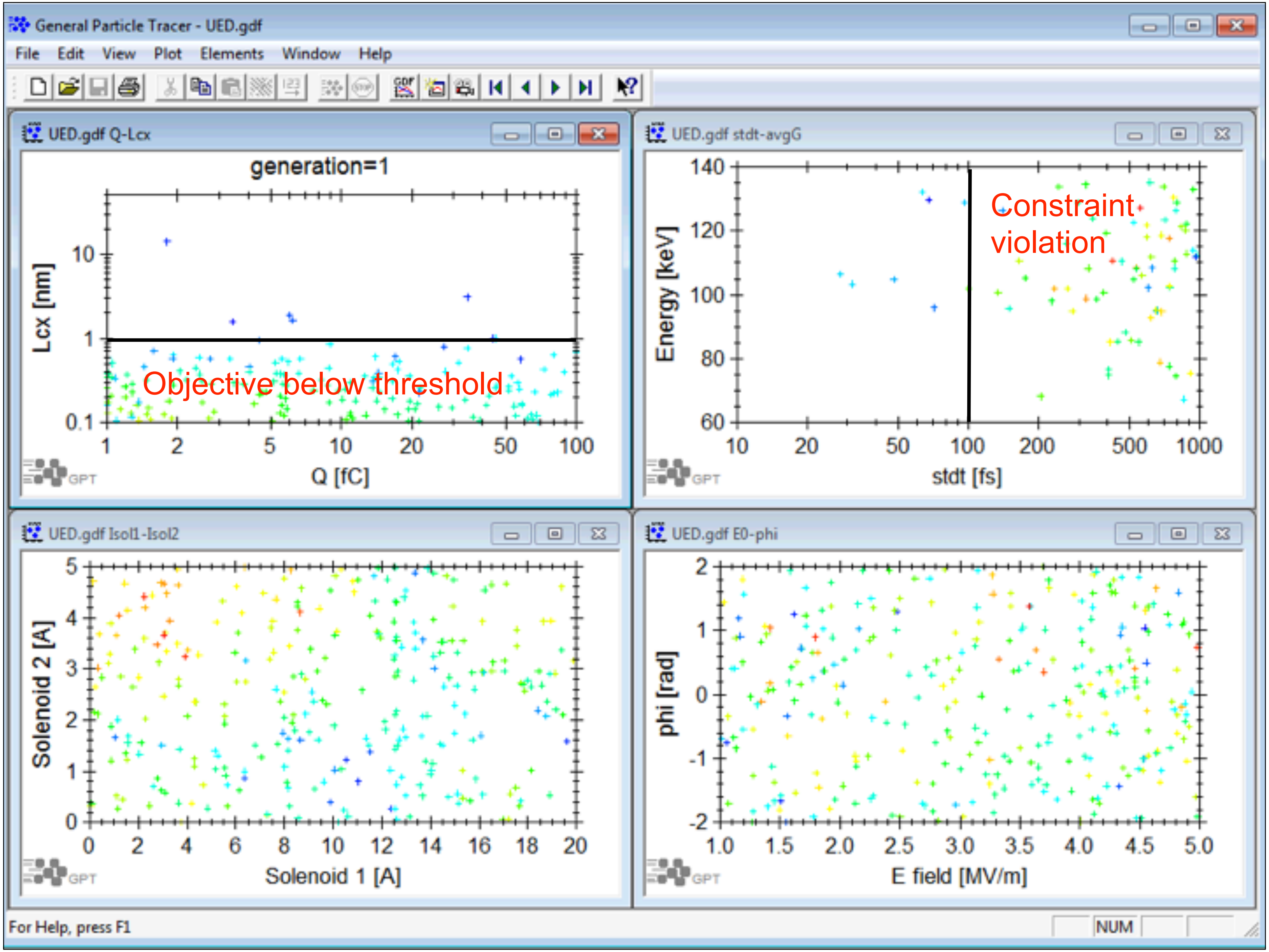
- **Structural dynamics**
- Resolve atomic **length** and **time scales**: ~1 Å, ~100 fs



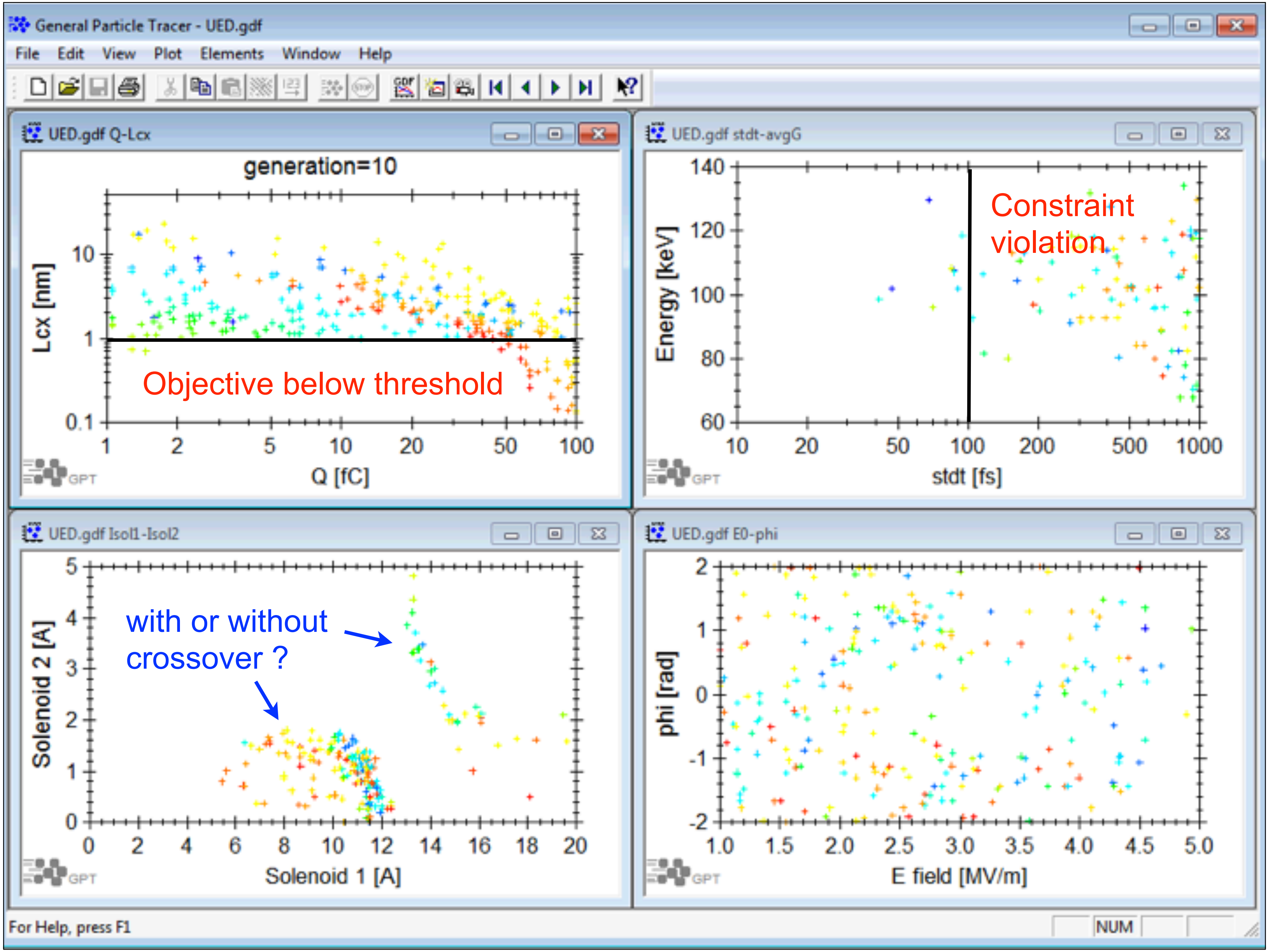
Example: Utrafast electron diffraction

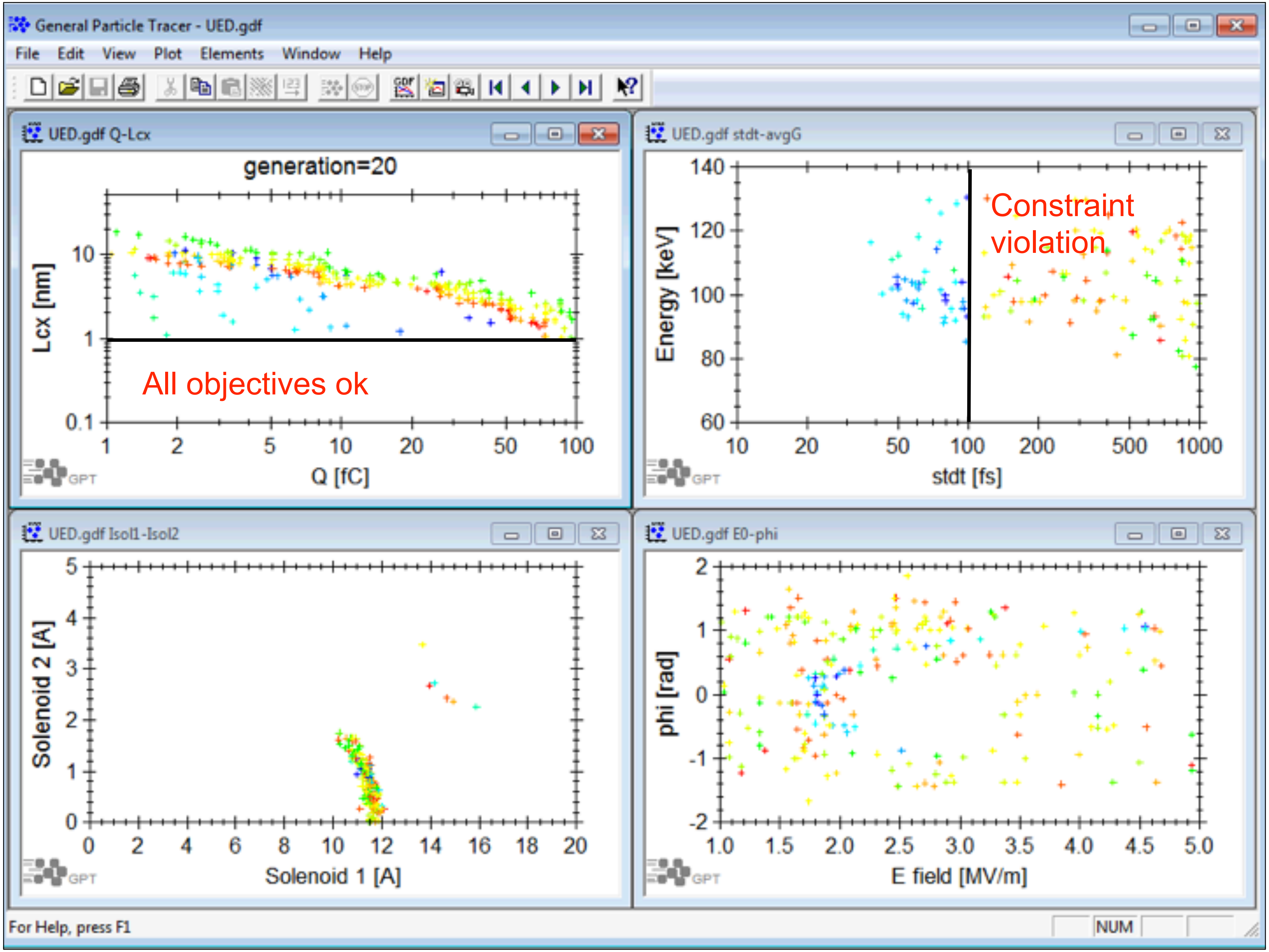
- **Variables: rf-amplitude, phase, solenoid1, solenoid2**
- **Conflicting objectives: Q, Lc>1 nm**
- **Constraints: pulse length≤100 fs, spot size≤250 μm**

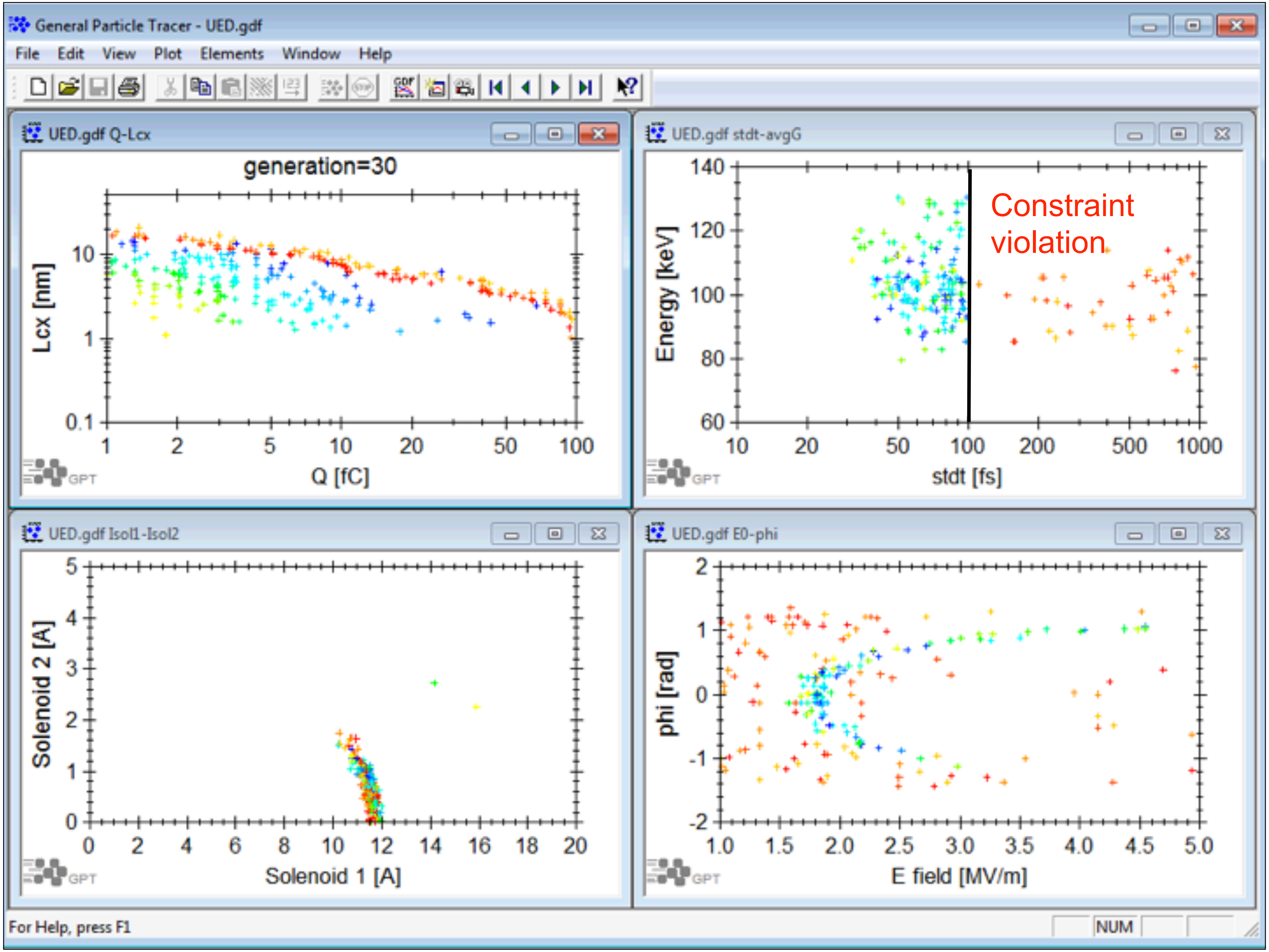




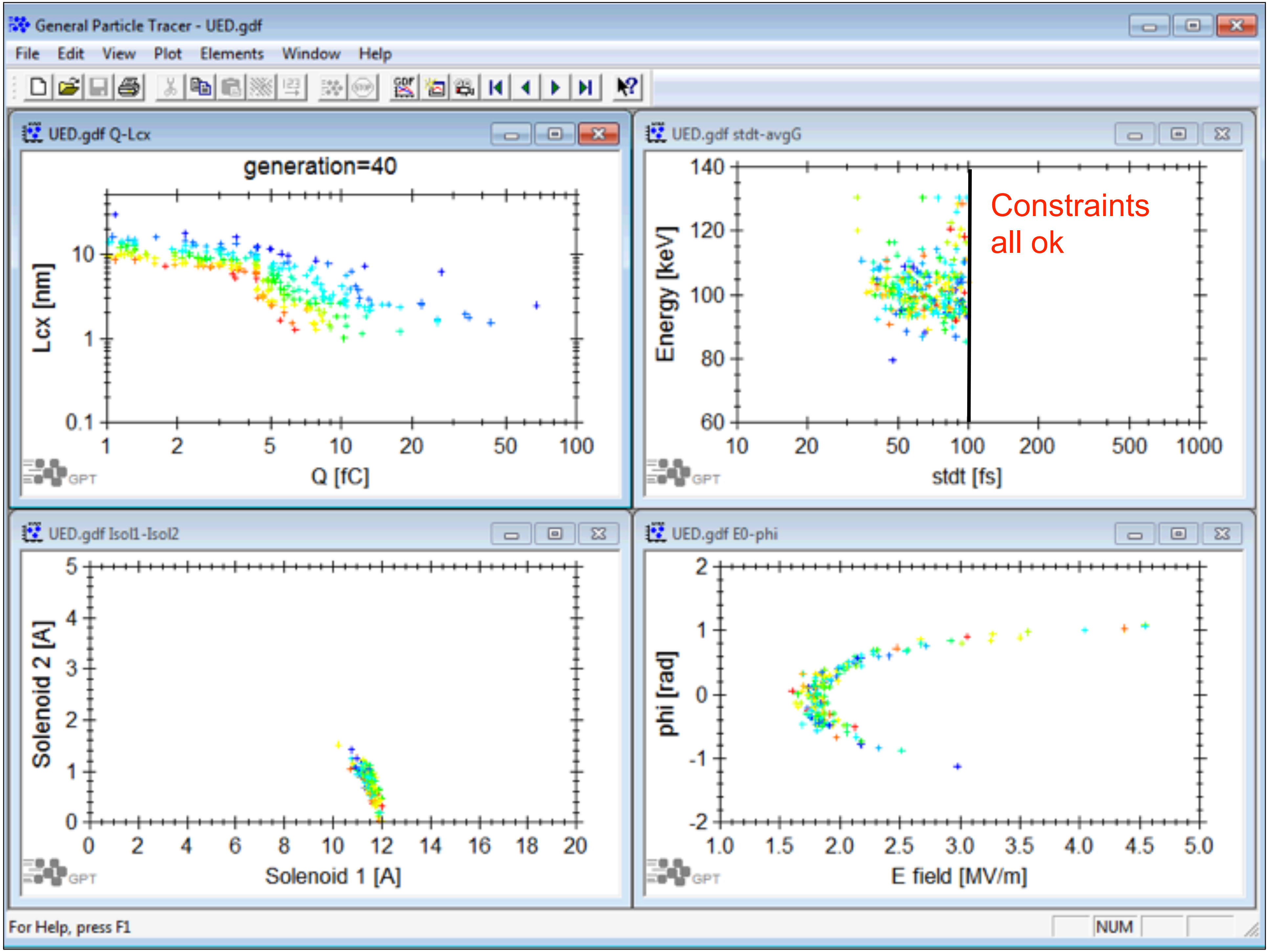
General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=1
Lcx [nm]
Q [fC]
Objective below threshold
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
Constraint violation
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM


General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=10
Lcx [nm]
Q [fC]
Objective below threshold
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
Constraint violation
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
with or without crossover ?
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM

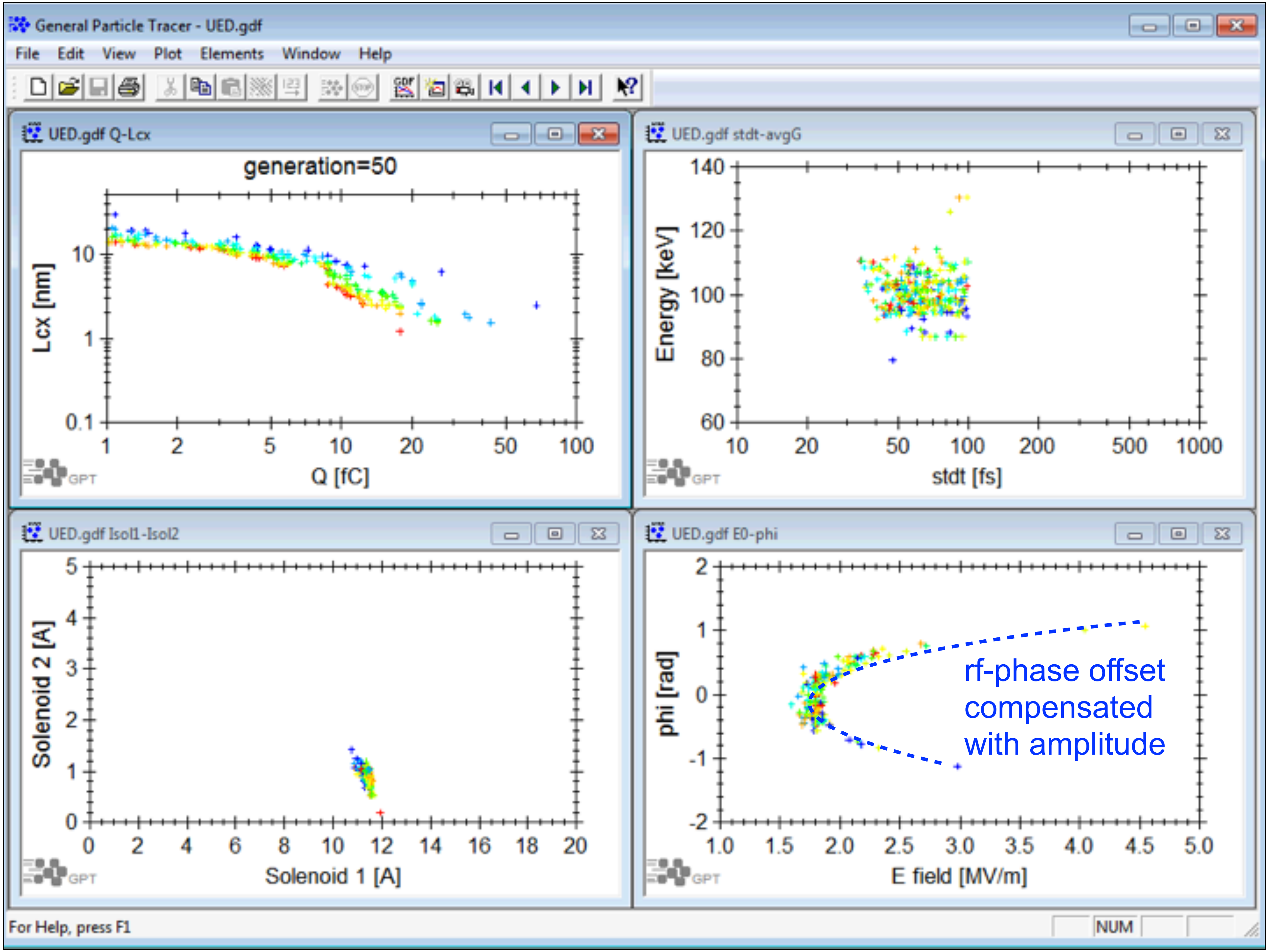

General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=20
Lcx [nm]
Q [fC]
All objectives ok
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
Constraint violation
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM

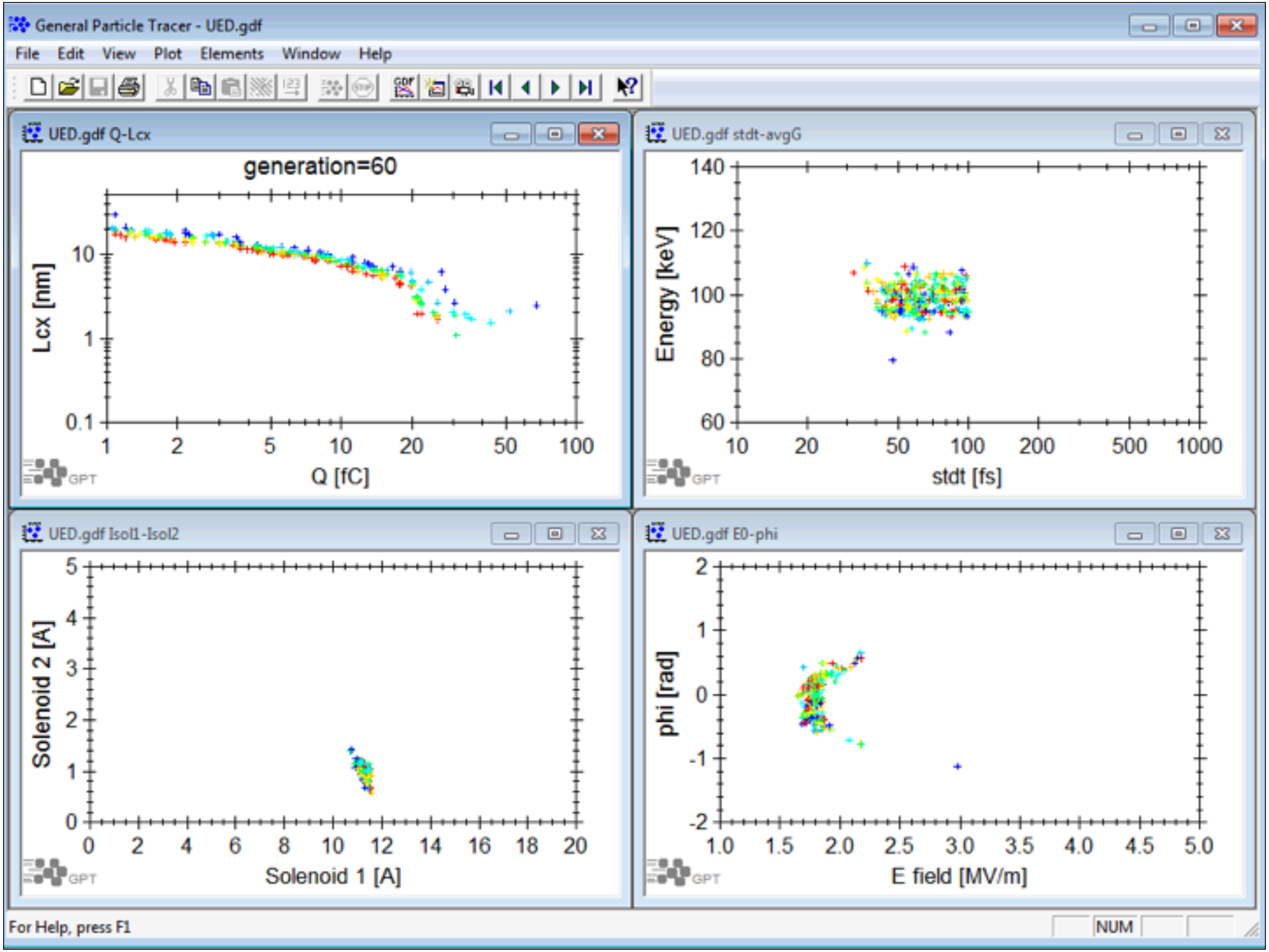


General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=30
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
Constraint violation
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM

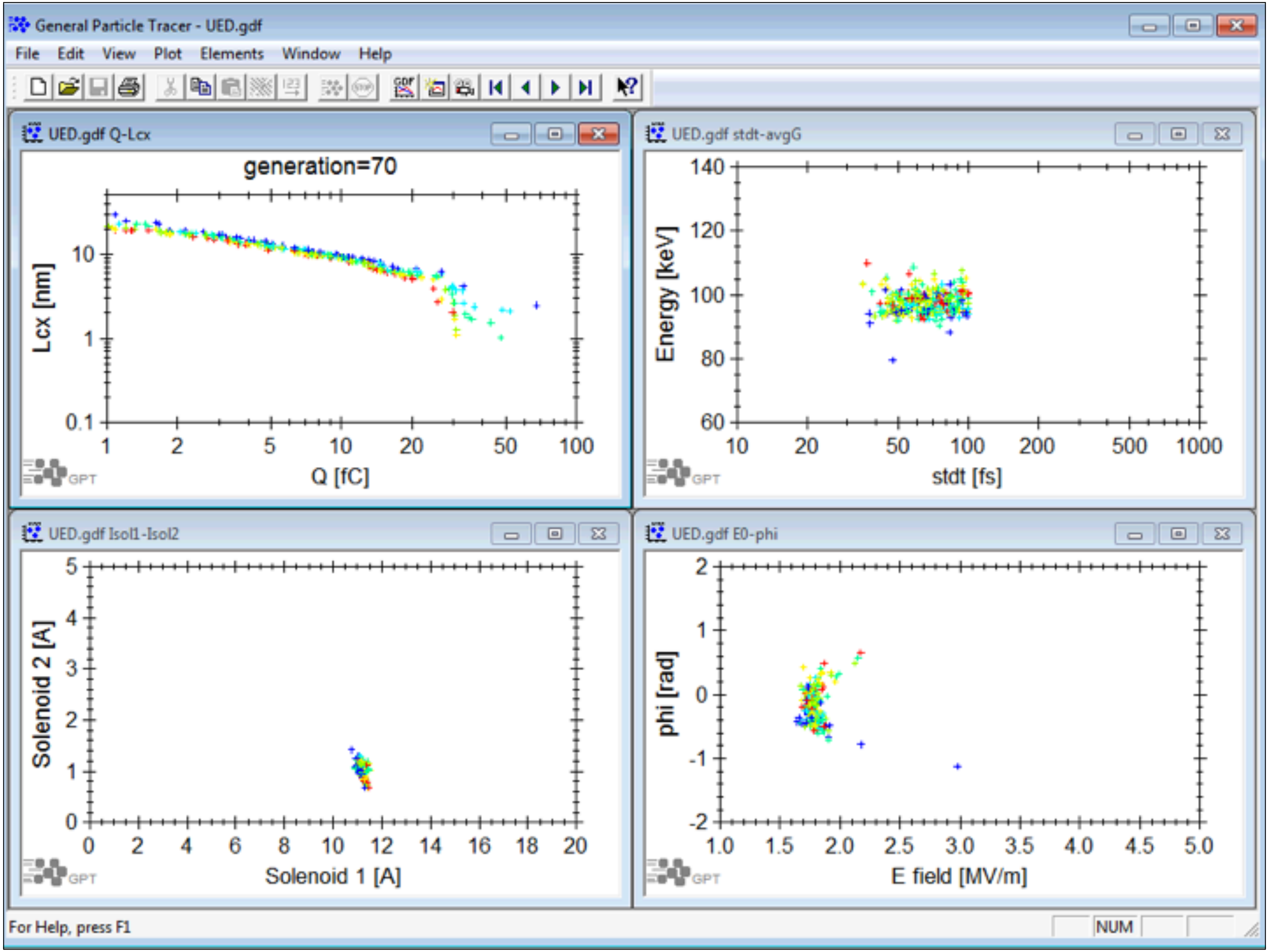


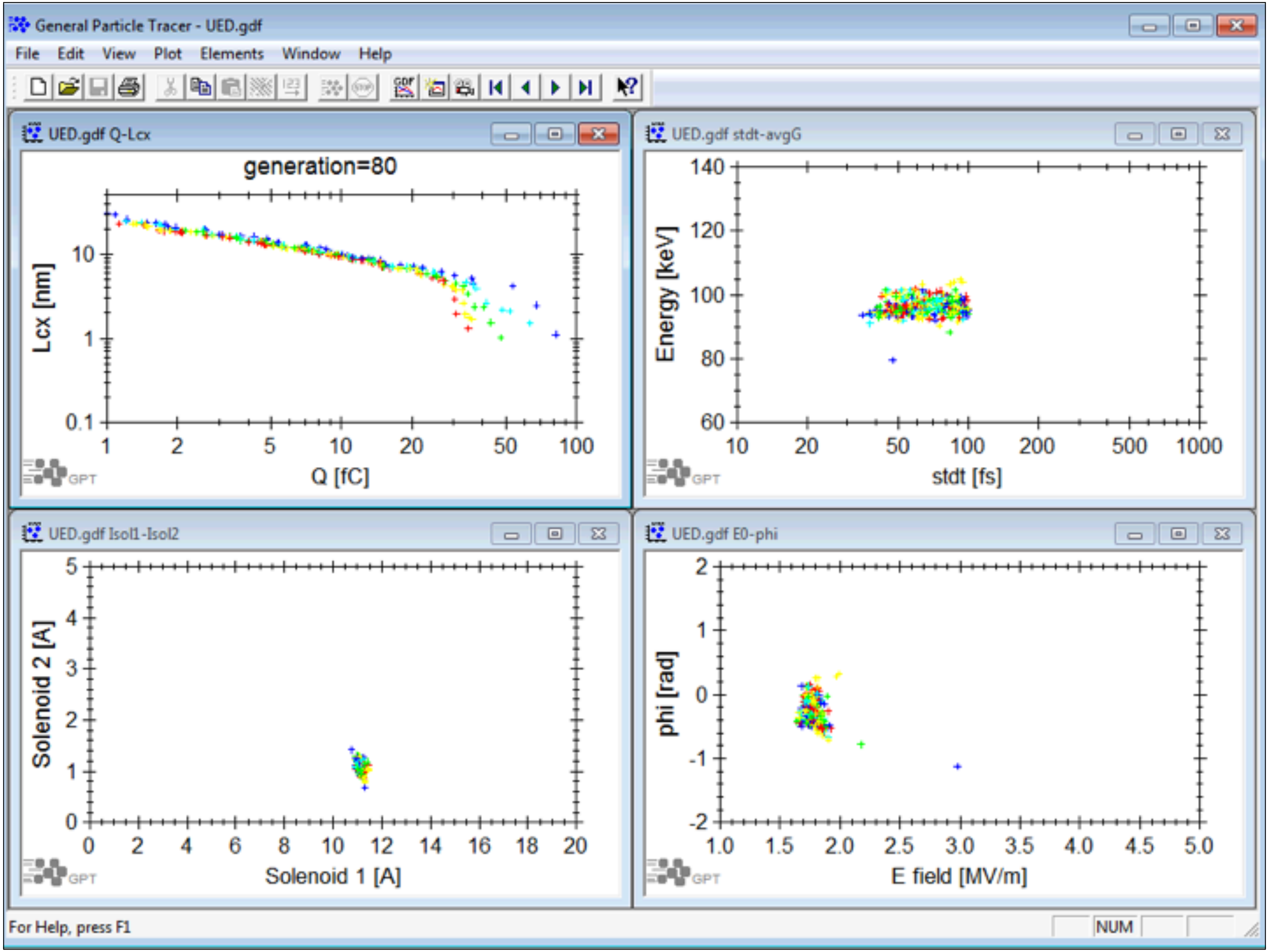
General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=40
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
Constraints
all ok
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM

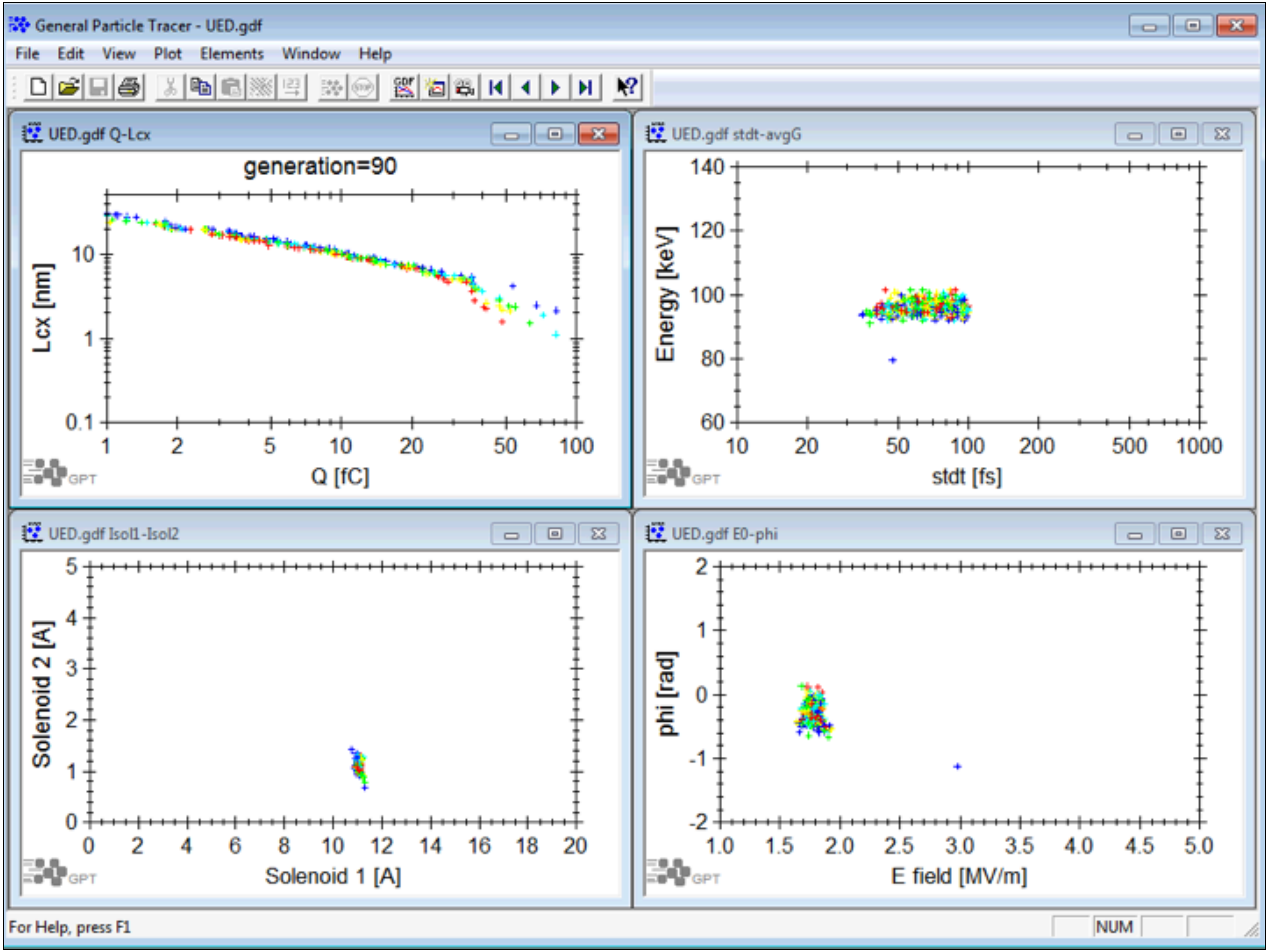

General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=50
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
rf-phase offset
compensated
with amplitude
For Help, press F1
NUM

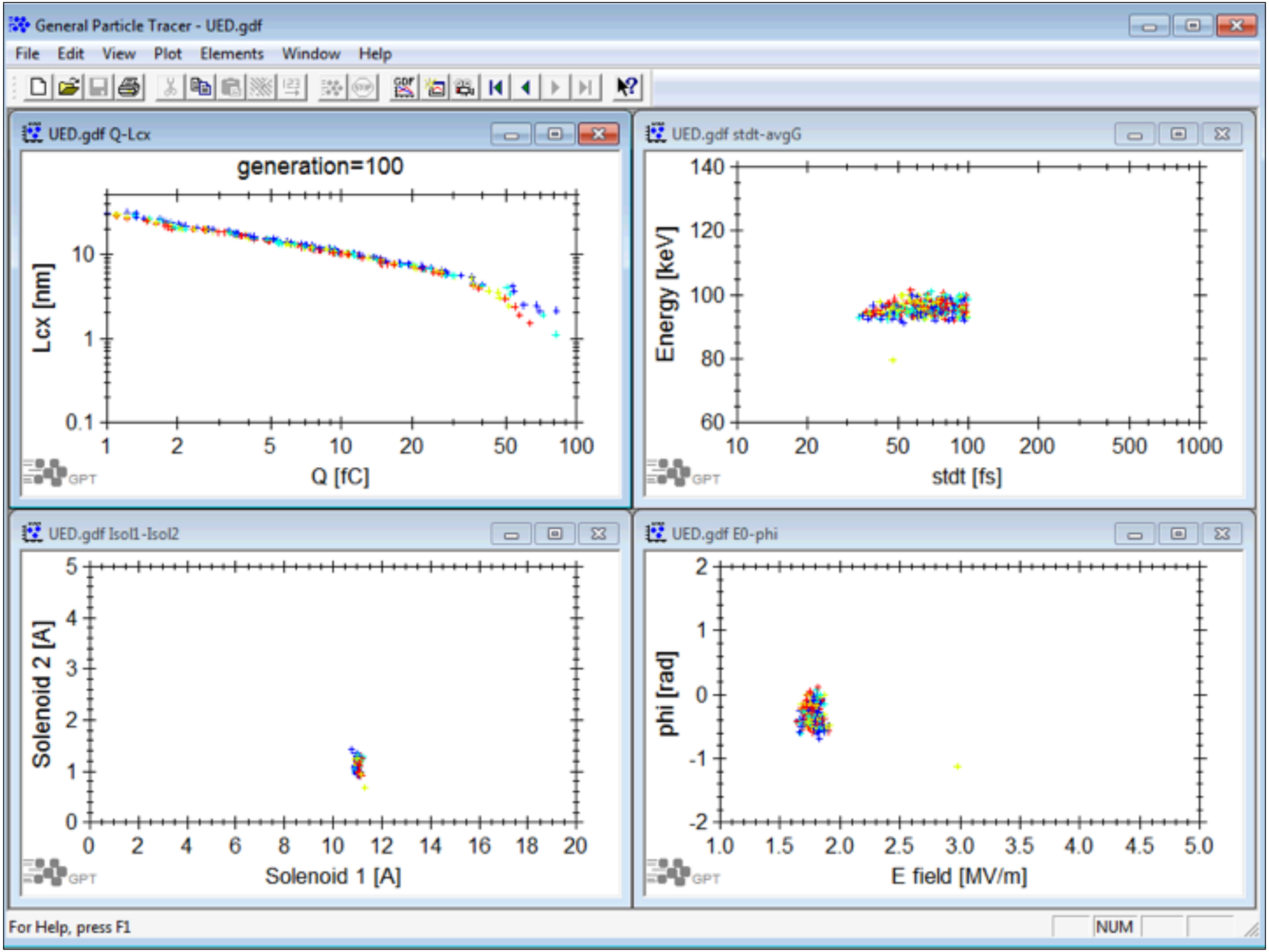


General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=60
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM

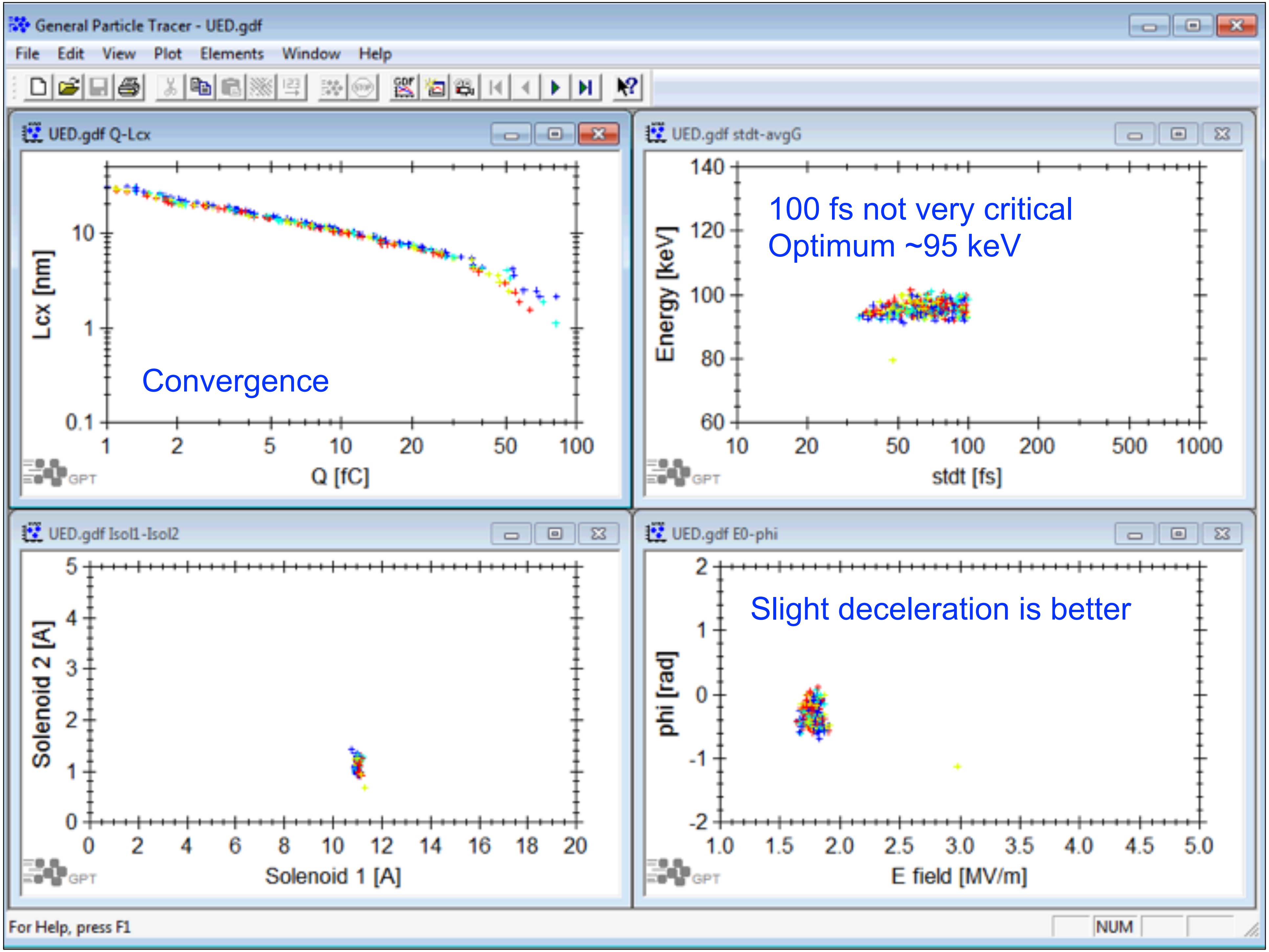

General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=70
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
GPT
For Help, press F1
NUM


General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=80
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
For Help, press F1
NUM


General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=90
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
GPT
For Help, press F1
NUM



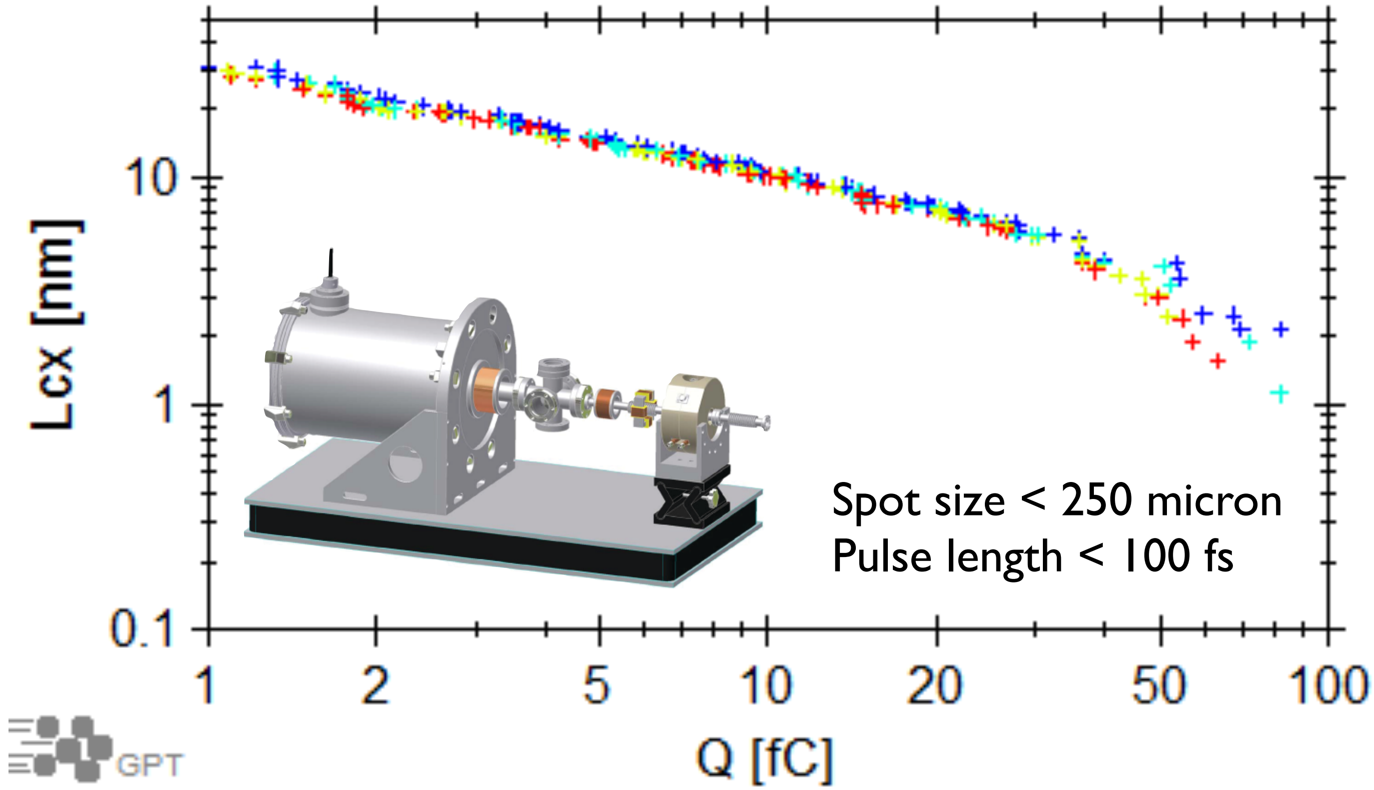
General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
generation=100
Lcx [nm]
Q [fC]
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
GPT
For Help, press F1
NUM



General Particle Tracer - UED.gdf
File Edit View Plot Elements Window Help
UED.gdf Q-Lcx
Lcx [nm]
Q [fC]
Convergence
UED.gdf stdt-avgG
Energy [keV]
stdt [fs]
100 fs not very critical
Optimum ~95 keV
UED.gdf Isol1-Isol2
Solenoid 2 [A]
Solenoid 1 [A]
UED.gdf E0-phi
phi [rad]
E field [MV/m]
Slight deceleration is better
For Help, press F1
NUM

Example: Utrafast electron diffraction

- **Variables: rf-amplitude, phase, solenoid1, solenoid2**
- **Conflicting objectives: Q, Lc**



Conclusion

Every design process has multiple objectives

Multi-objective genetic optimization (MGO):

- **Fully automates the design process**
- **Gives trade-offs, not ‘best’ solutions**
- **Relatively insensitive to local minima**
- **Can handle additional constraints**
- **Requires robust simulation tools (such as GPT)**

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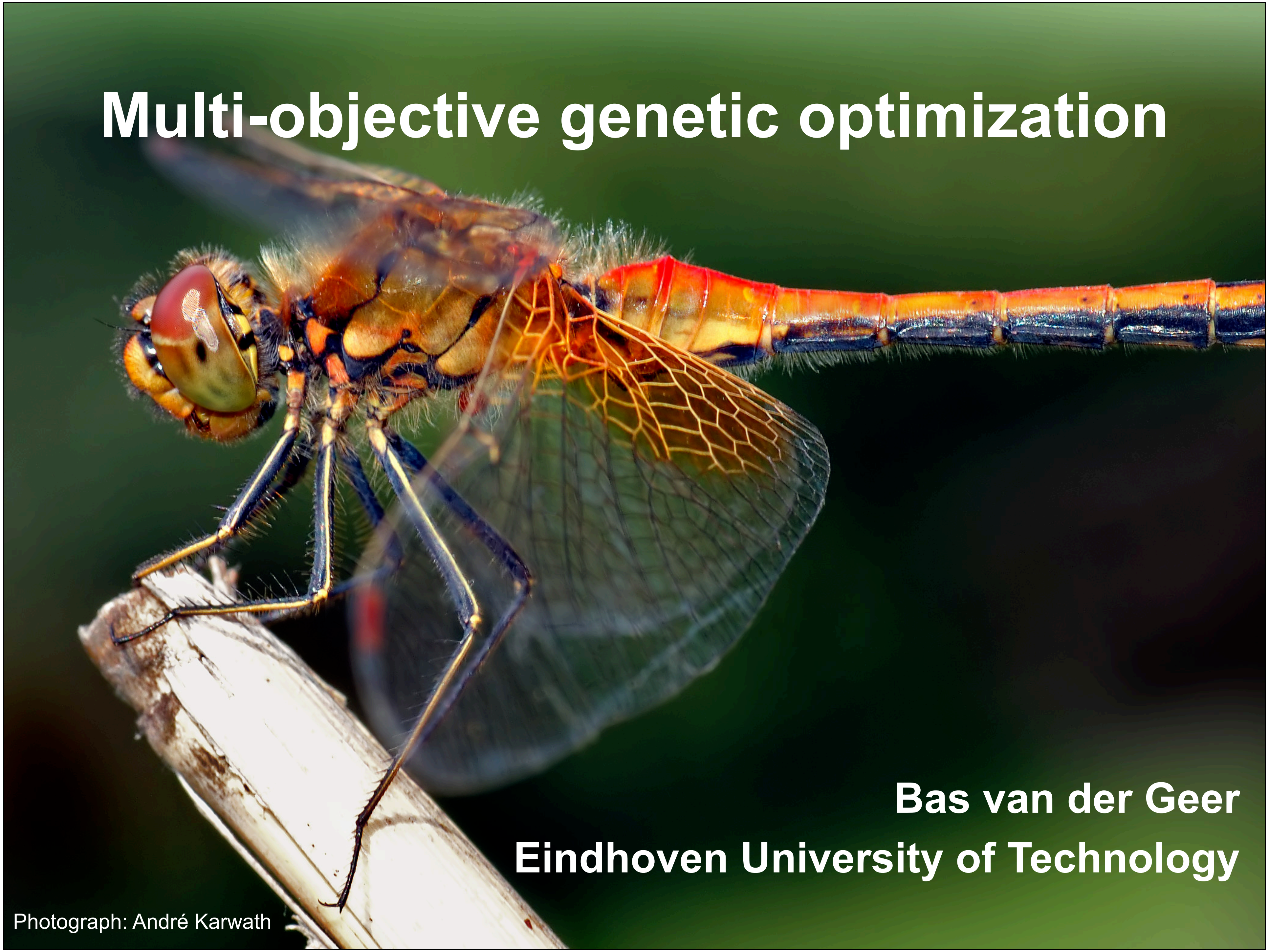
AND

MGO is a perfect match with a multi-core supercomputer

Multi-objective genetic optimization



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Photograph: André Karwath