# A Surrogate Model to Optimize Injection Efficiency in PSI muEDM Experiment

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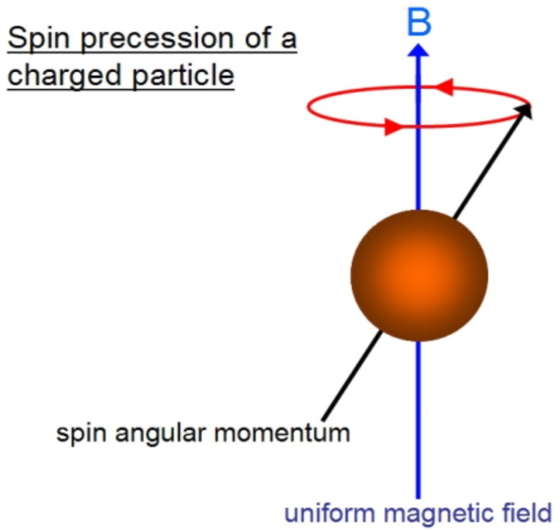
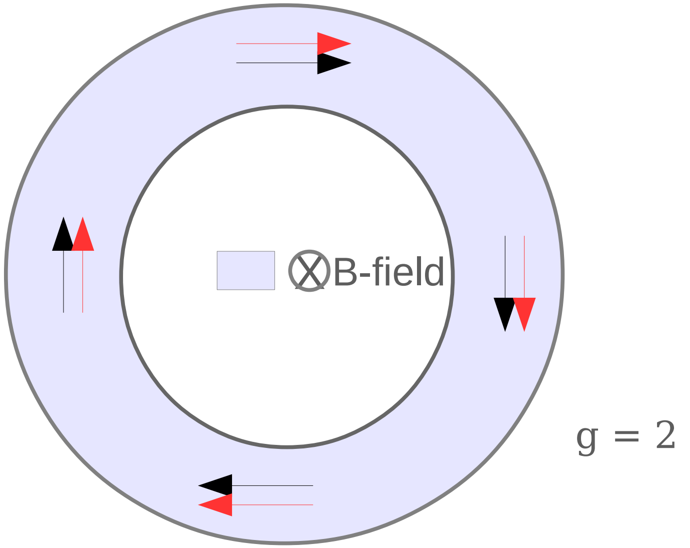
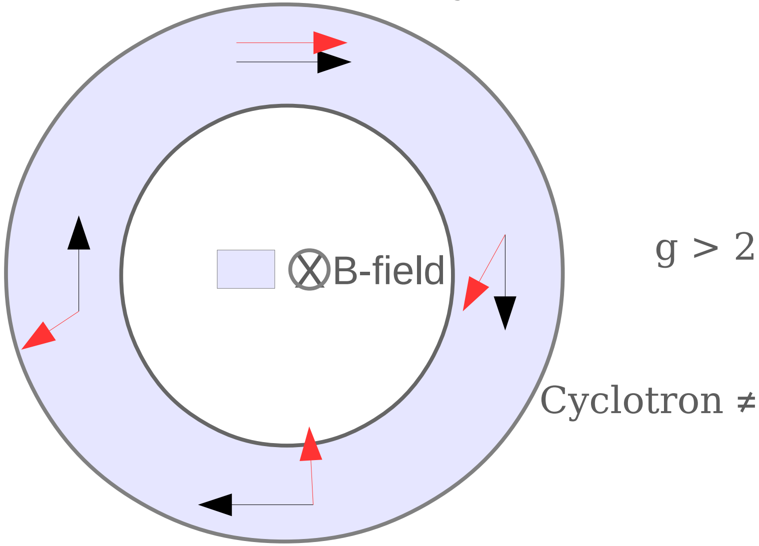
# Muons in a Storage Ring




Cyclotron = spin precession

In presence of vacuum effects:




Cyclotron ≠ spin precession

# Muons Electric Dipole Moment (EDM)

In general, relativistic muons, in presence of electric fields + magnetic field

$$\vec{\Omega} = \vec{\Omega}_0 - \vec{\Omega}_c$$

Spin precession      Cyclotron

Thomas-BMT equation for spin dynamics in EM fields:

$$\vec{\Omega} = \underbrace{\frac{q}{m}\left[a\vec{B} - \frac{a\gamma}{(\gamma+1)}\left(\vec{\beta}\cdot\vec{B}\right)\vec{\beta} - \left(a + \frac{1}{1-\gamma^2}\right)\frac{\vec{\beta}\times\vec{E}}{c}\right]}_{\text{g-2 term}} + \underbrace{\frac{\eta q}{2m}\left[\vec{\beta}\times\vec{B} + \frac{\vec{E}}{c} - \frac{\gamma c}{(\gamma+1)}\left(\vec{\beta}\cdot\vec{E}\right)\vec{\beta}\right]}_{\text{EDM term}}$$

- Non-zero muon EDM indicates CP-violation
- Standard model prediction ~$10^{-38}$ e.cm
- PSI muon EDM sensitivity target 6 x $10^{-23}$ e.cm → ~3 order of magnitude better than current limit

# Frozen Spin Technique

- $E \perp B \perp \beta$

$$\vec{\Omega} = \frac{q}{m}\left[a\vec{B} - \frac{a\gamma}{(\gamma+1)}(\vec{\beta}\cdot\vec{B})\vec{\beta} - \left(a + \frac{1}{1-\gamma^2}\right)\frac{\vec{\beta}\times\vec{E}}{c}\right] + \frac{\eta q}{2m}\left[\vec{\beta}\times\vec{B} + \frac{\vec{E}}{c} - \frac{\gamma c}{(\gamma+1)}(\vec{\beta}\cdot\vec{E})\vec{\beta}\right]$$

g-2 term

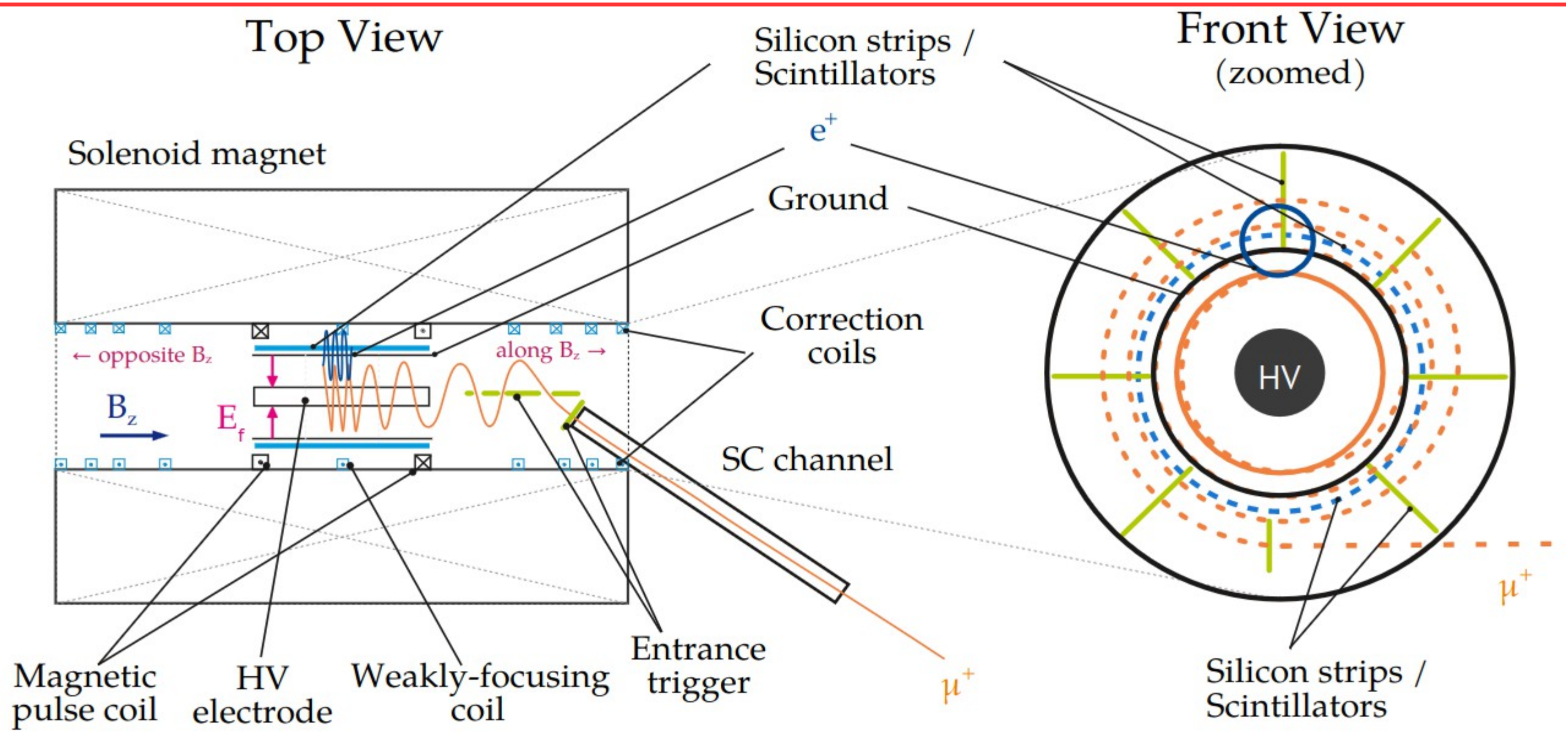
EDM term

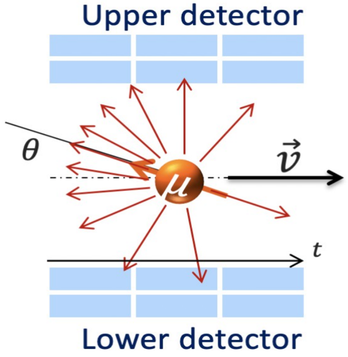
- Suppress g-2 term by setting $a\vec{B} = \left(a - \frac{1}{\gamma^2 - 1}\right)\frac{\vec{\beta}\times\vec{E}}{c}$
- Radial E-field $E_f \approx aBc\beta\gamma^2$

$$\vec{\omega}_e = \frac{\eta q}{2m}\left[\vec{\beta}\times\vec{B} + \frac{\vec{E}_f}{c}\right]$$

Precession frequency only due to EDM

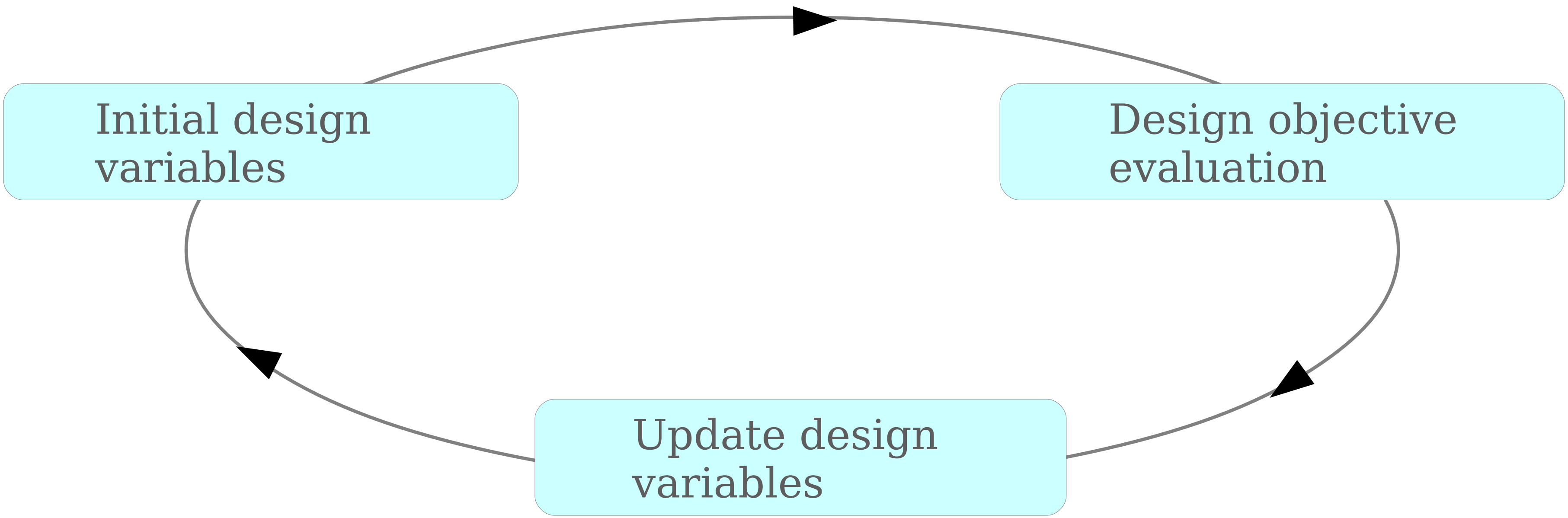
# PSI muEDM Experiment



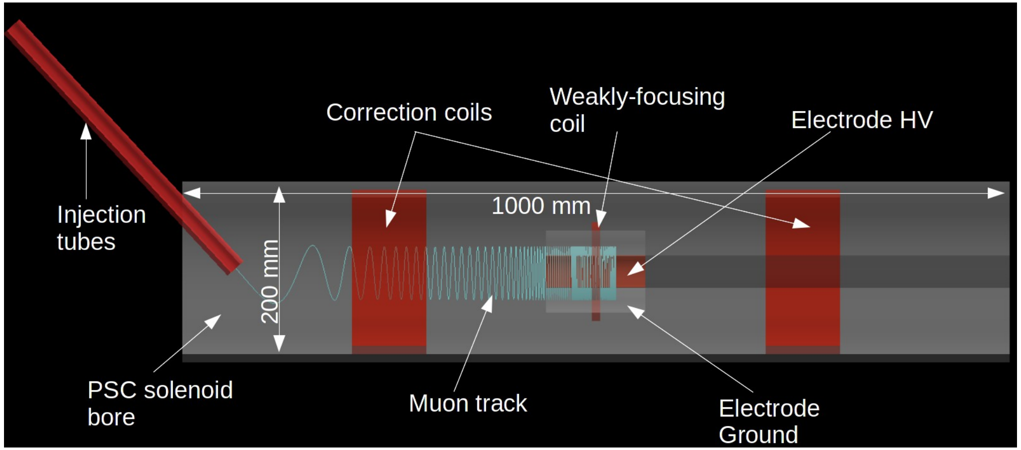

Asymmetry in number of detected positrons upstream vs downstream is proportional to EDM signal

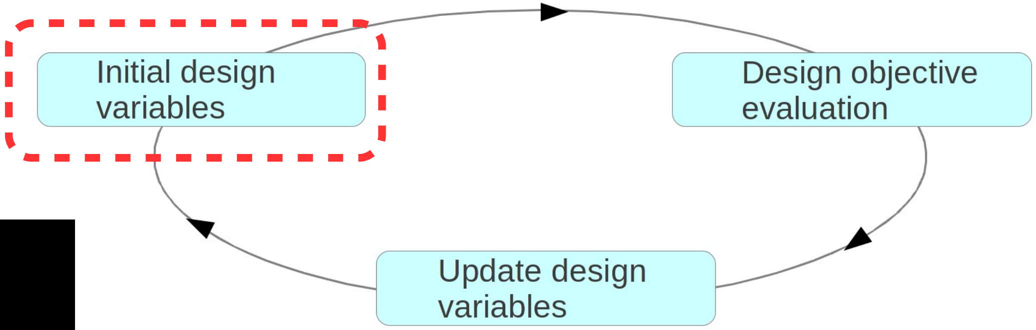
# Design Optimization Layout

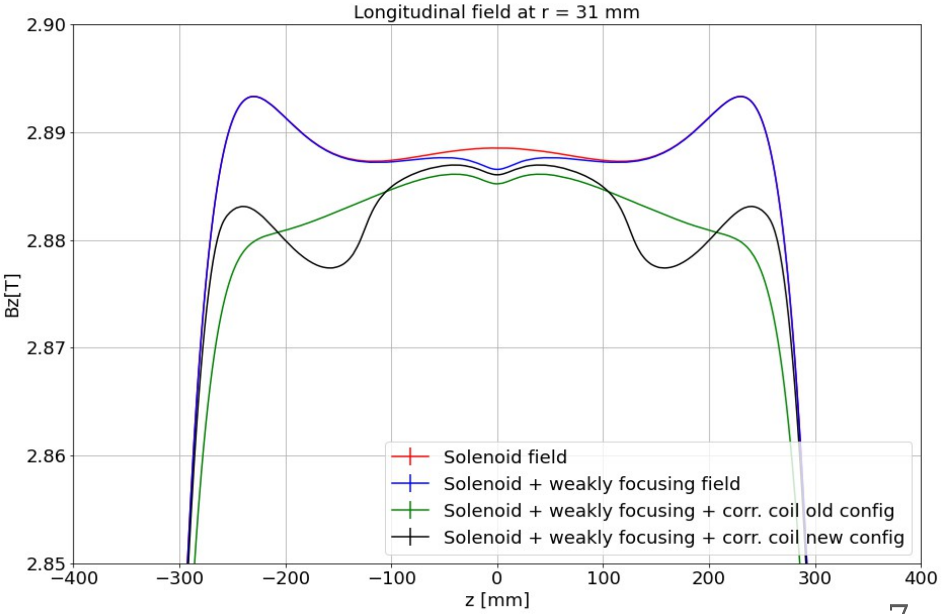


# Design Optimization Layout

Design simulation in g4bl



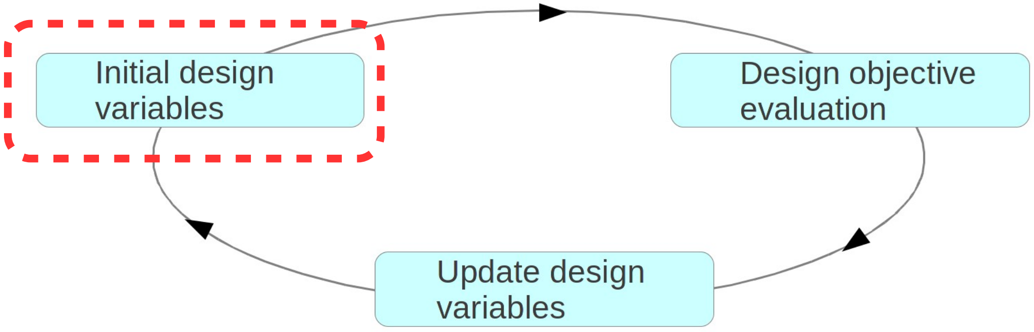



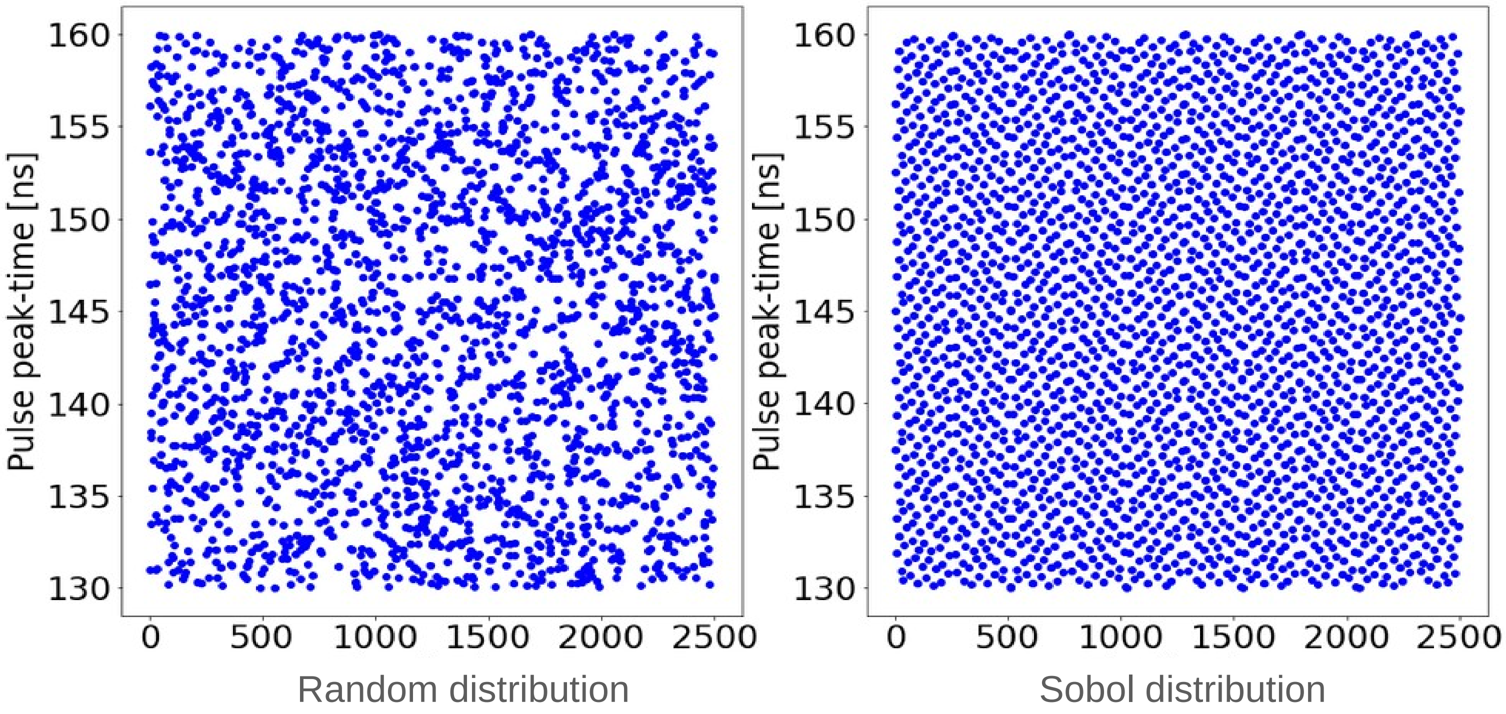

Design parameters:

- Injection coordinates
- Magnetic field strength
- Correction coil features
- Weak-focusing coil features
- Kicker pulse features
- ……

# Design Optimization Layout

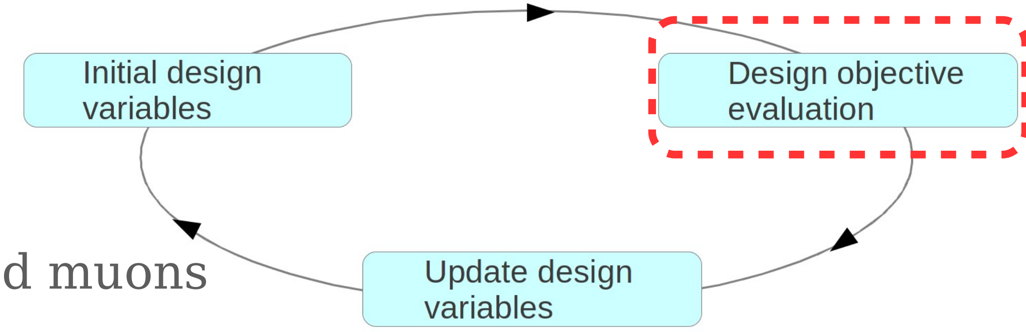
- Sampling input variables
- Sobol distribution *(Sobol, 1967)*
- Maximum uniform spread

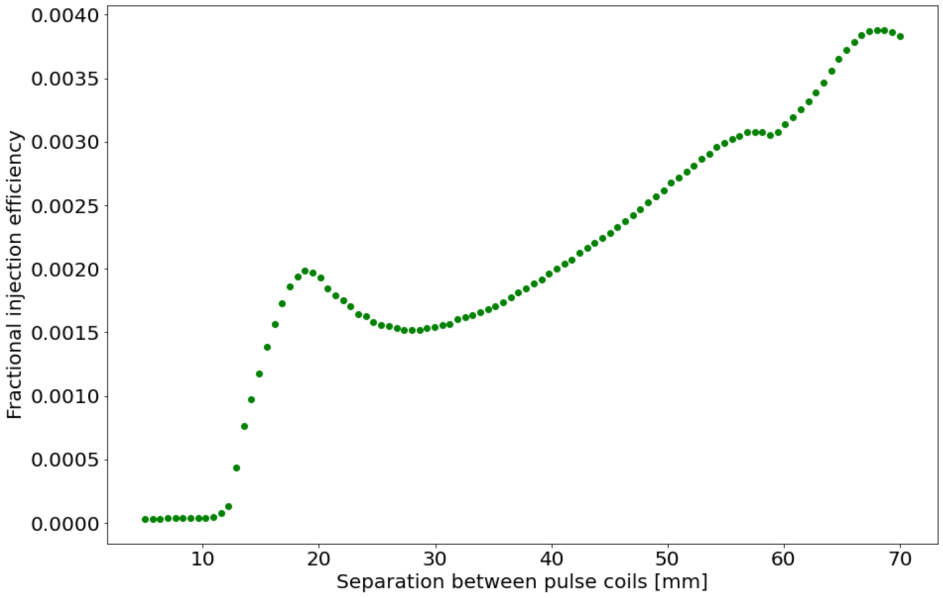


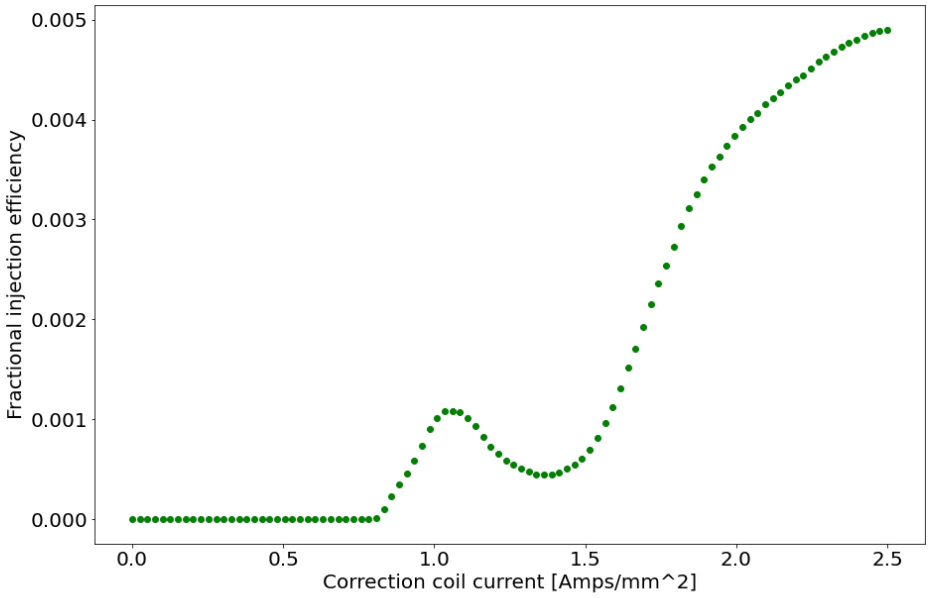



# Design Optimization Layout

- Maximize injection efficiency
- Minimize power dissipation of setup
- Minimize polarization spread in stored muons
- ....

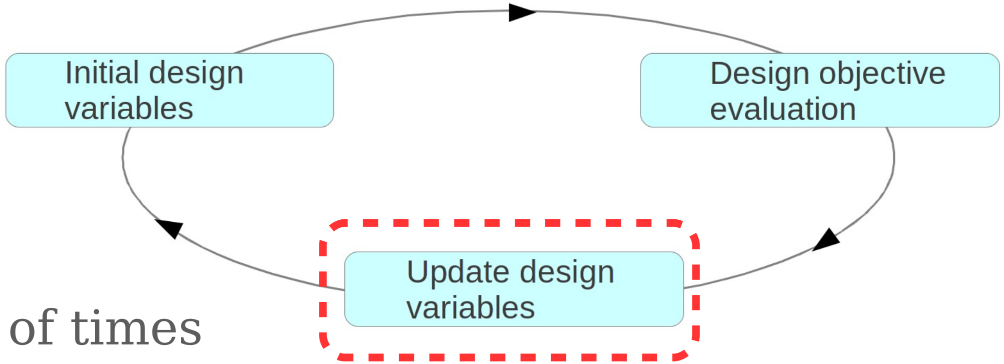


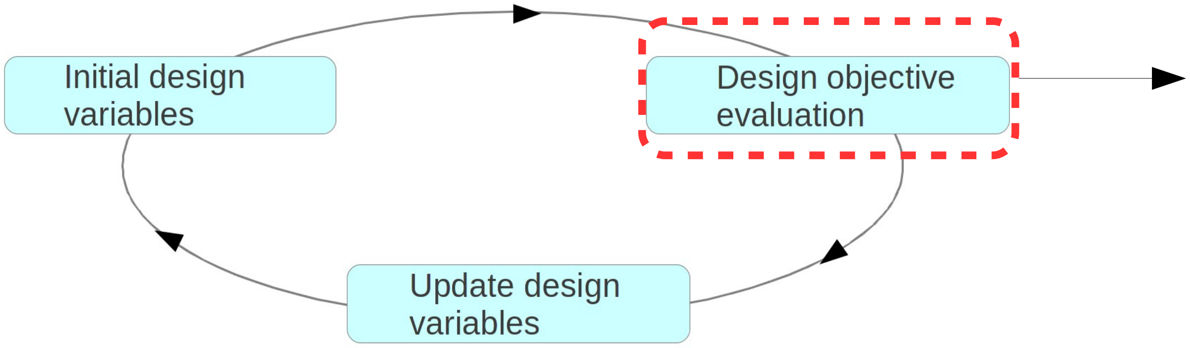



# Design Optimization Layout

- Update design variables based on objective evaluation
- Repeat until optimal solution found
- Required to run simulation thousands of times → computationally expensive
- Replace physics simulation with approximation → surrogate model




Surrogate model for objective evaluation
→ Many ways
→ PCE and NN models explored

# PCE Surrogate Model

- Polynomial Chaos Expansion (PCE) :

$$Y = \sum_{i=0}^{\infty} \alpha_i \Psi_i(\vec{x})$$

$\boldsymbol{Y}$ → Model response (injection efficiency), $\boldsymbol{\Psi_i}$ → Orthogonal polynomials
x → input variables, $\boldsymbol{\alpha_i}$ → expansion coefficients

- Polynomial basis based on input variable distribution

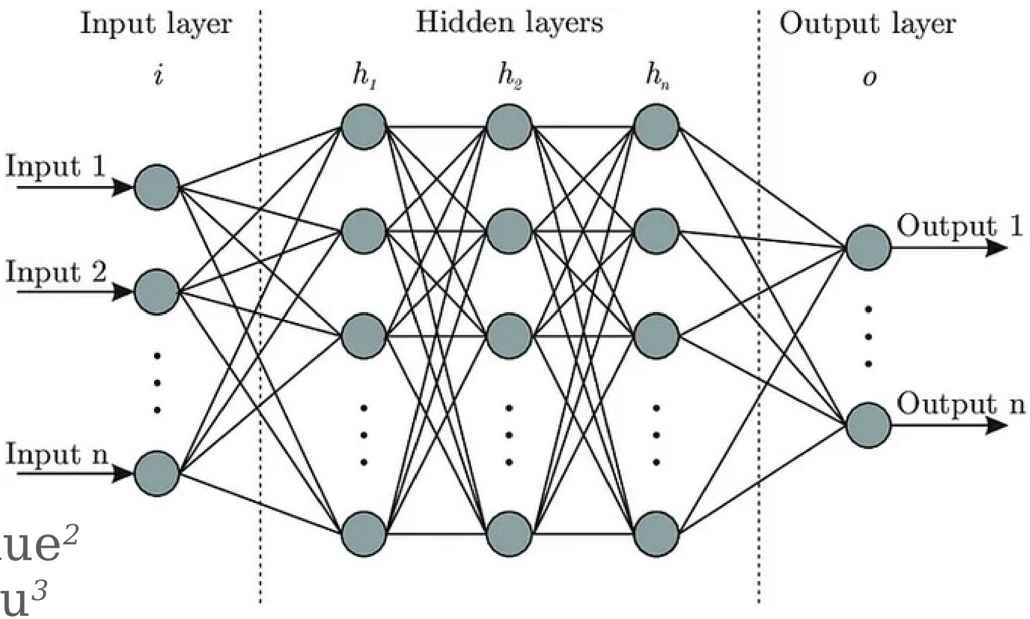
- Coefficients determined using regression based methods

$$\vec{\alpha} = \text{Argmin}\frac{1}{N}\sum_{j=1}^{N}\left\{f(\vec{\xi}^j) - \sum_{i=0}^{P-1}\alpha_i\Psi_i(\vec{x}^j)\right\}^2$$

# NN Surrogate Model

- Use the input (design) and output (objective) to train a neural network

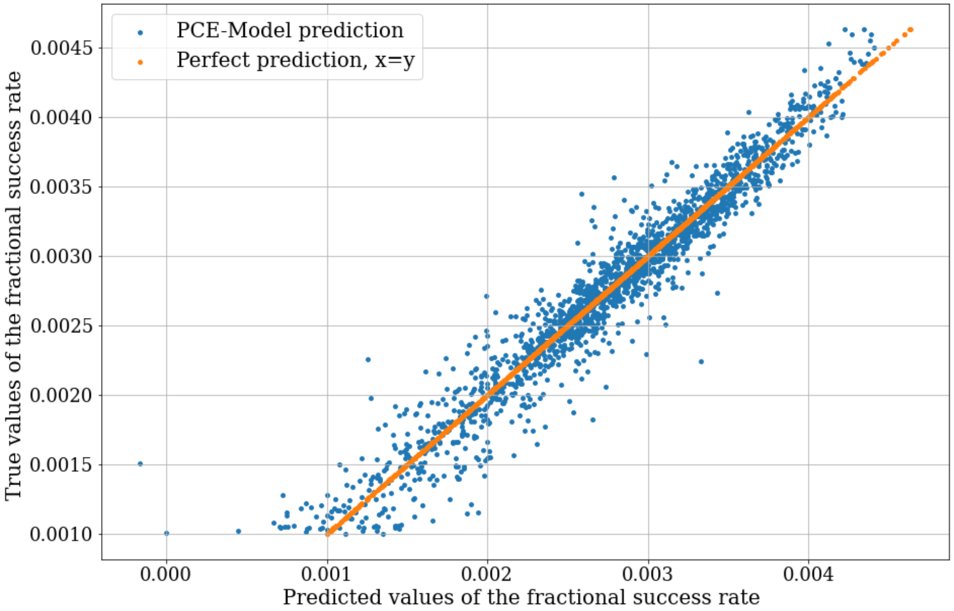
- Hyper parameters:
  → no. of hidden layers = 8
  → no. of neurons/layer = 500
  → learning rate = 0.001
  → optimizer: Adam[1]
  → scheduler: ReduceLRonPlateaue[2]
  → activation function: LeakyReLu[3]



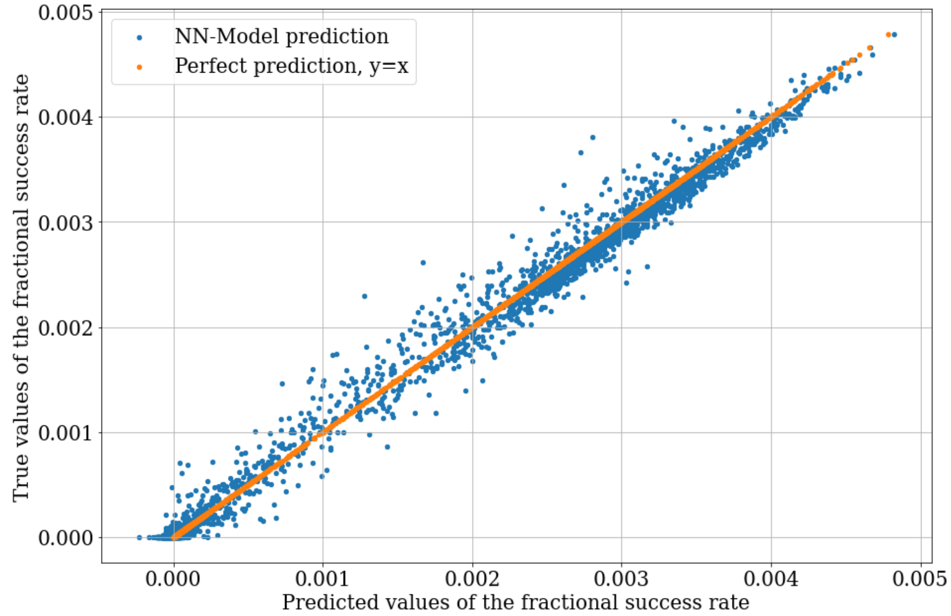

[1] *Kingma and Ba, 2014* [2] *Maas, 2013* [3] *K Developers, 2019*

# Surrogate Model Performance

Model performance for a 6 dimensional input space
(Kicker timing, Kicker strength, Corr coil position, Corr coil length, Corr coil thickness and Corr coil radius)

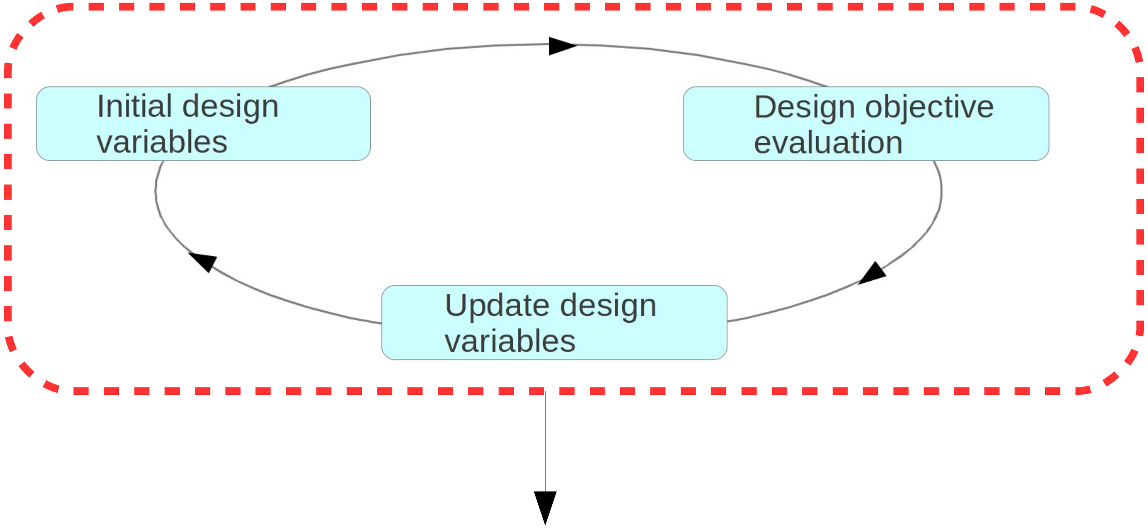



PCE Mean Square Error: 3.47 e-08



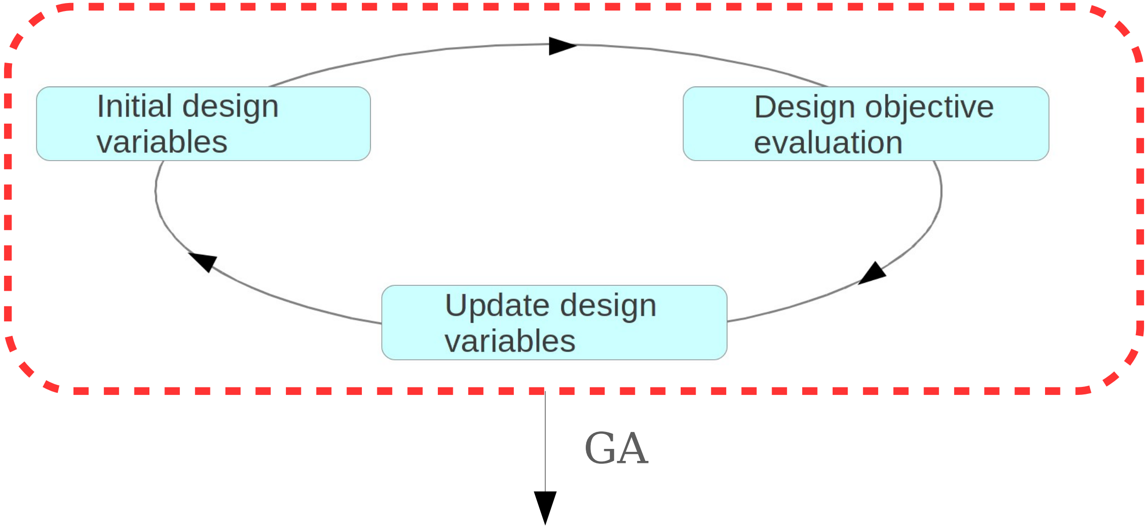

NN Mean Square Error: 1.88 e-08

# Multi-objective Optimization



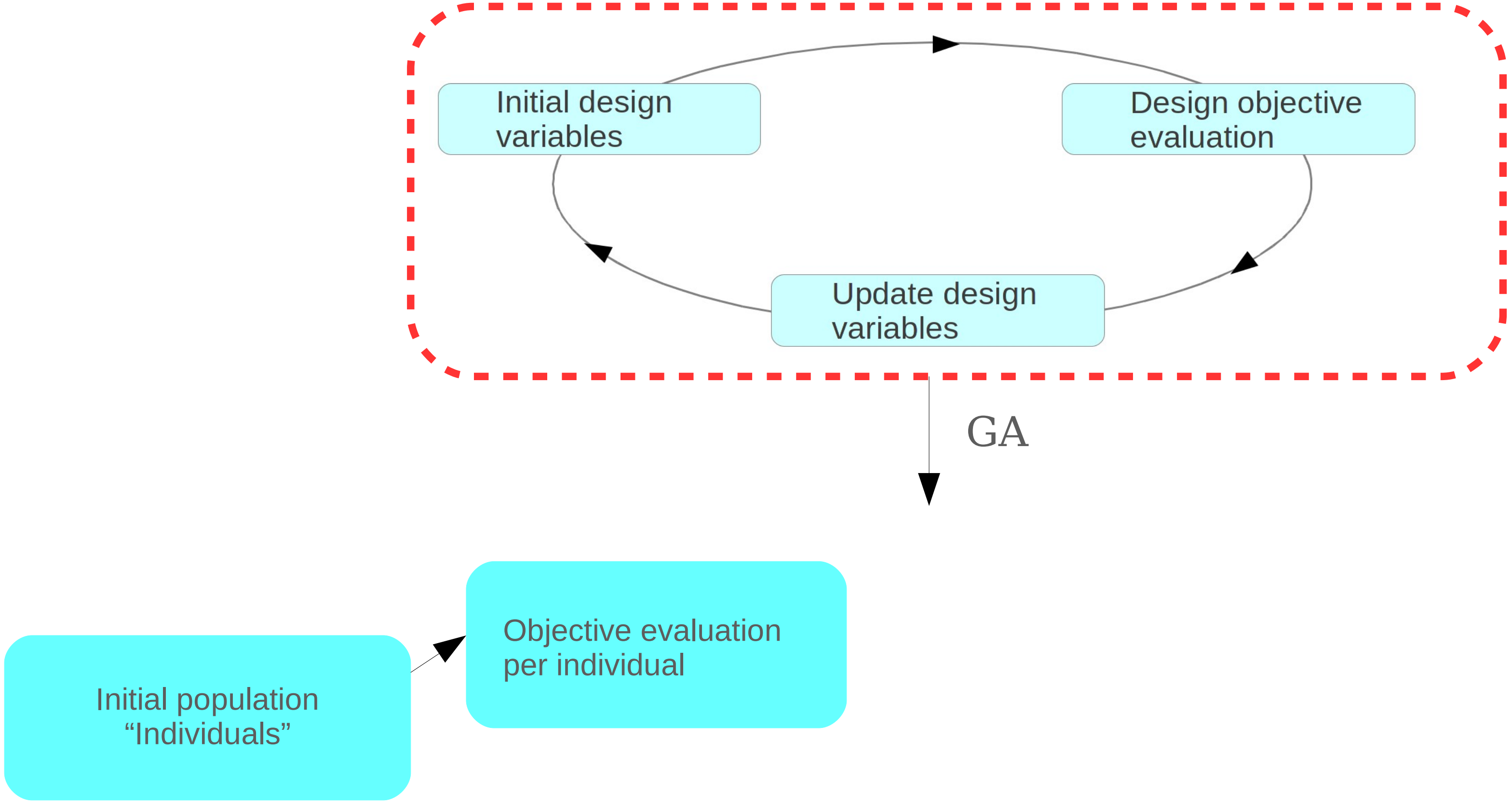

Genetic Algorithms (GA)

# Genetic Algorithm

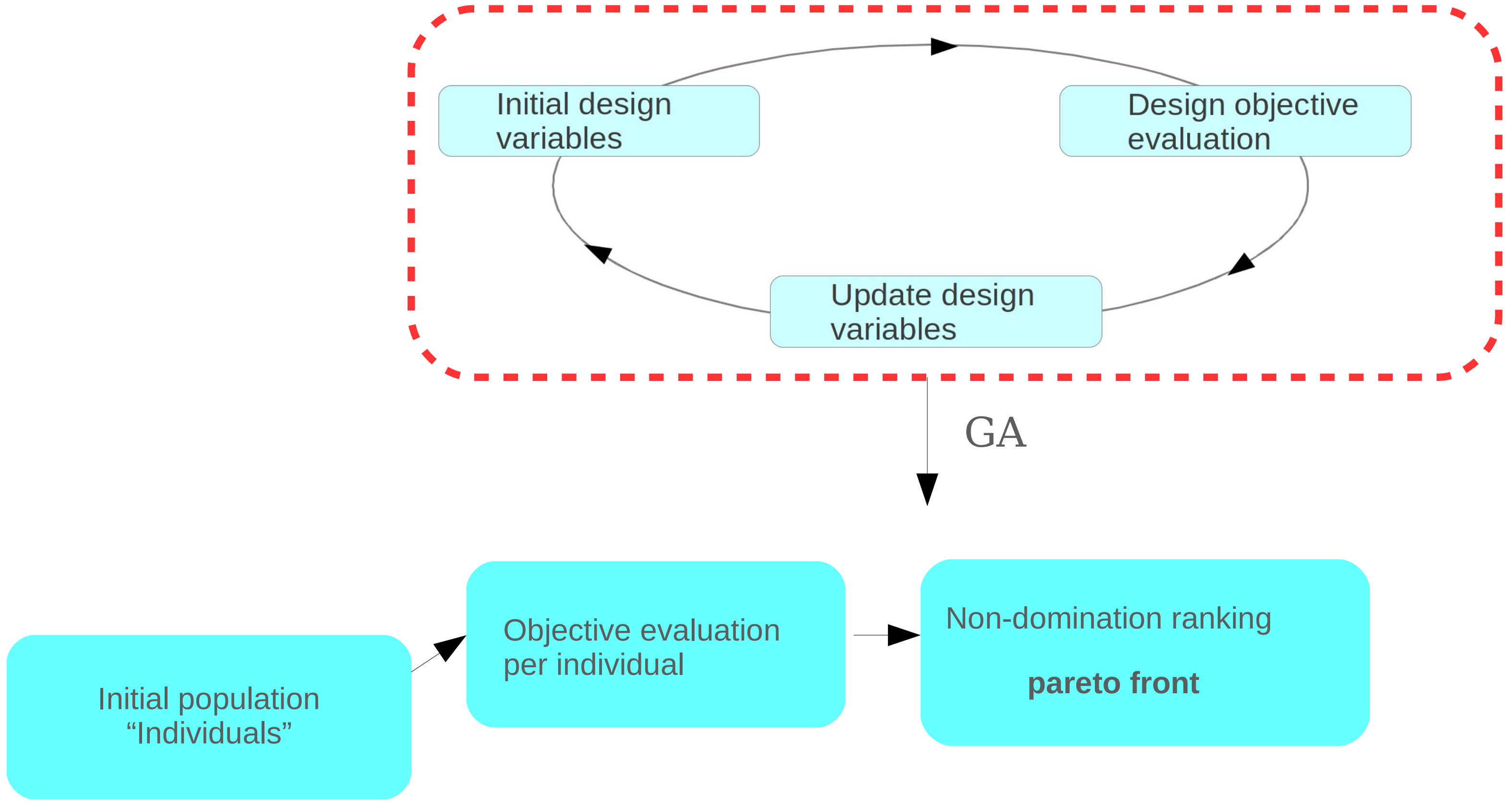



Initial population
“Individuals”

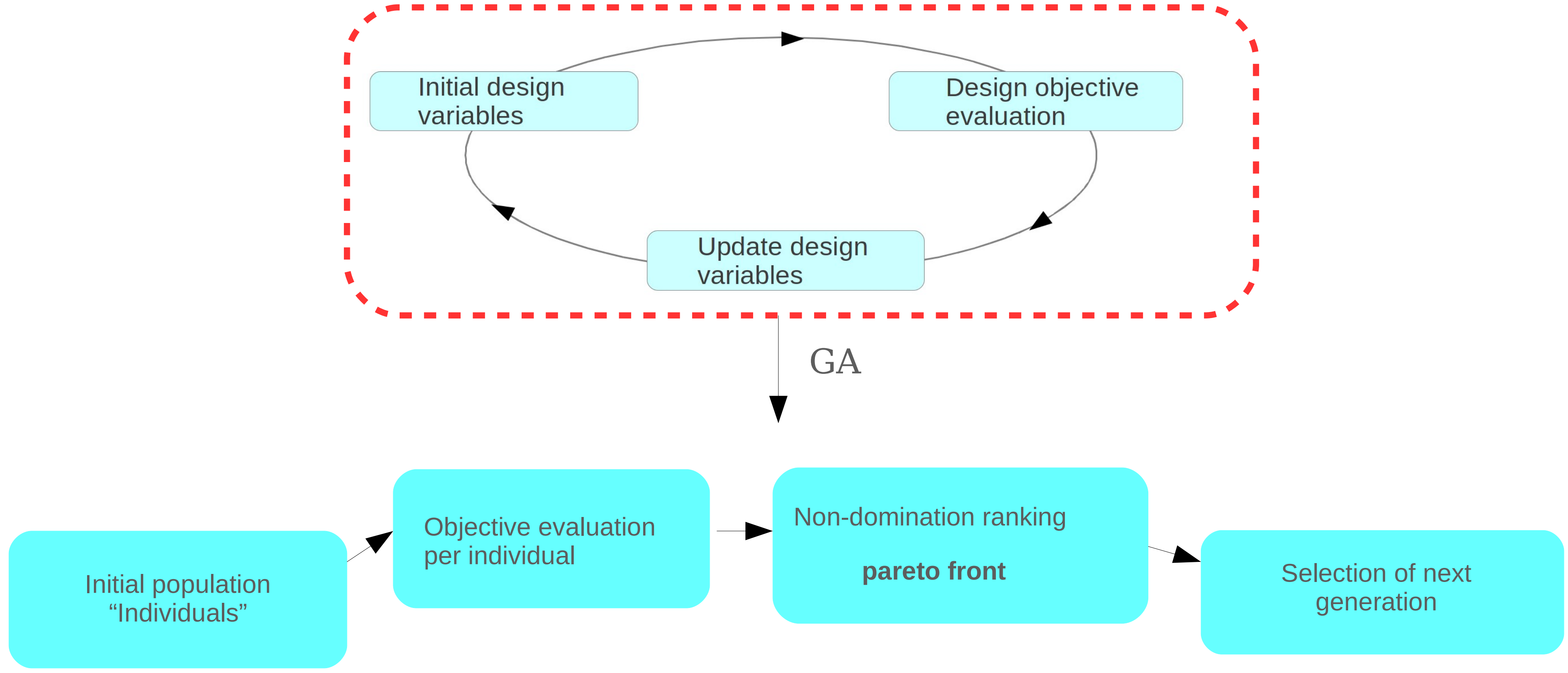
# Genetic Algorithm



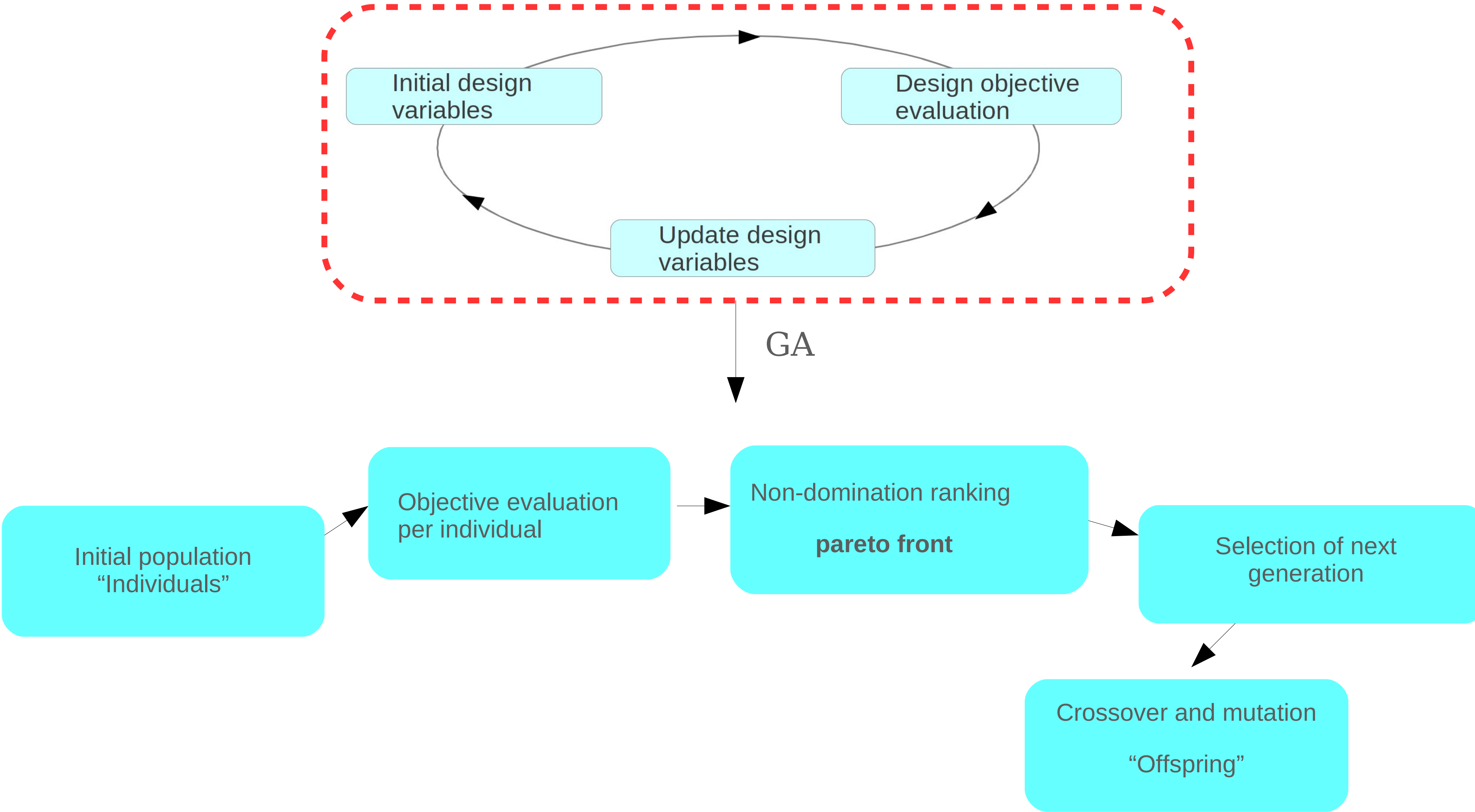
# Genetic Algorithm



# Genetic Algorithm



# Genetic Algorithm



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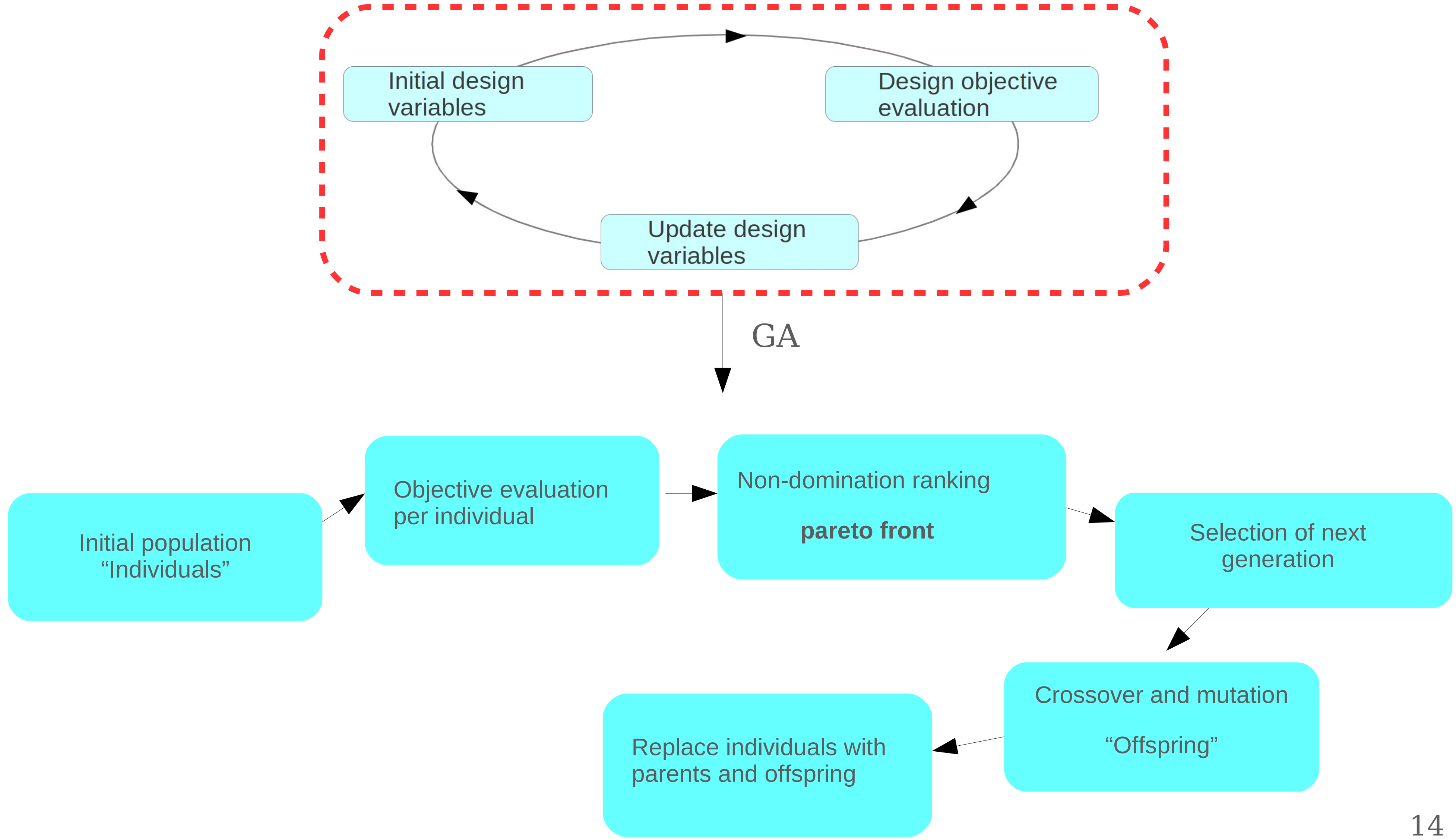
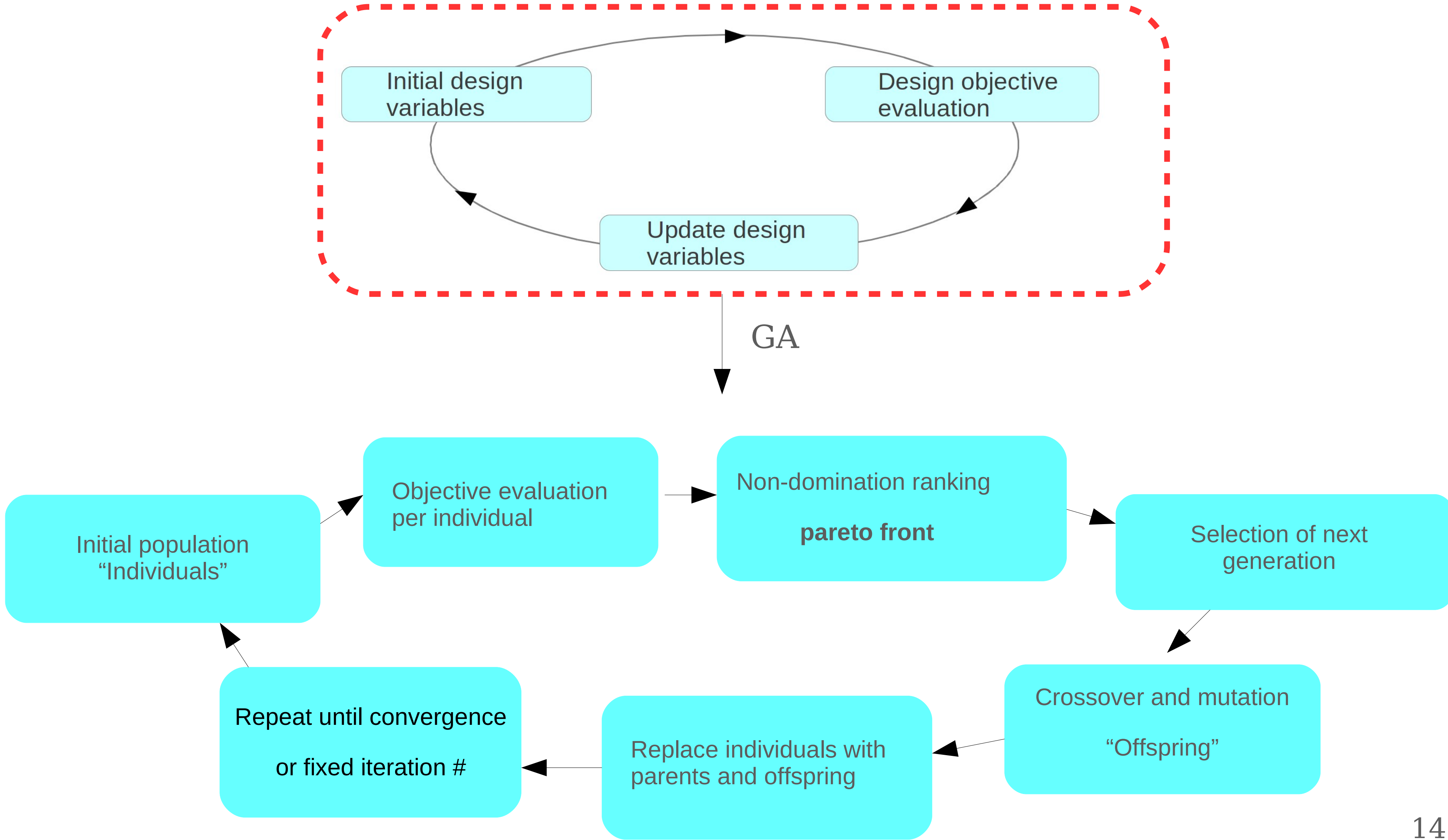
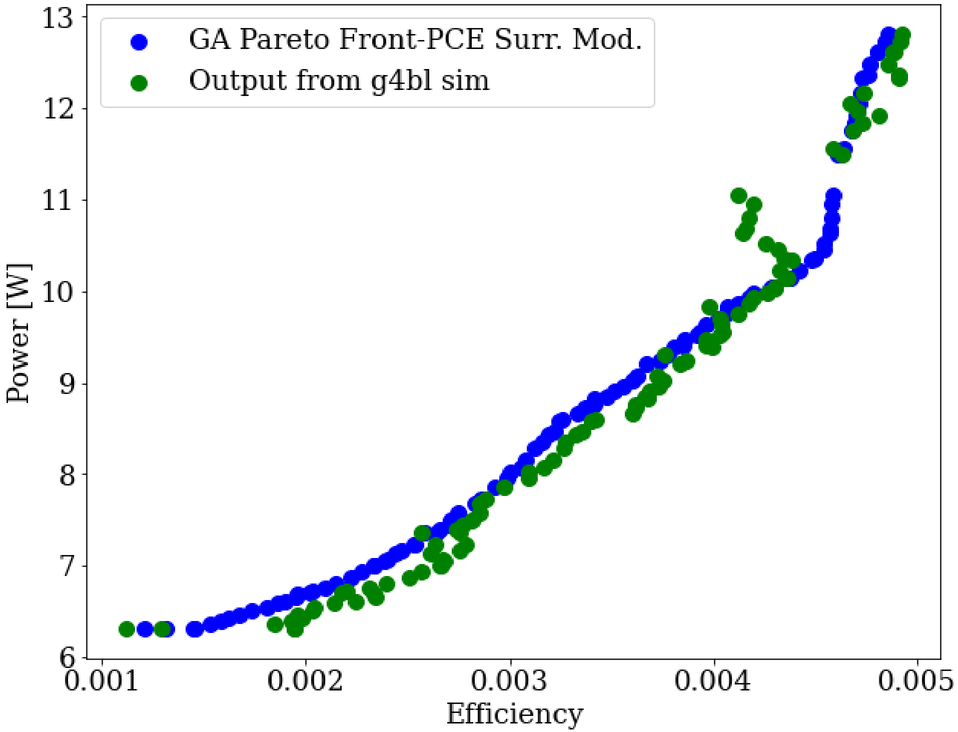


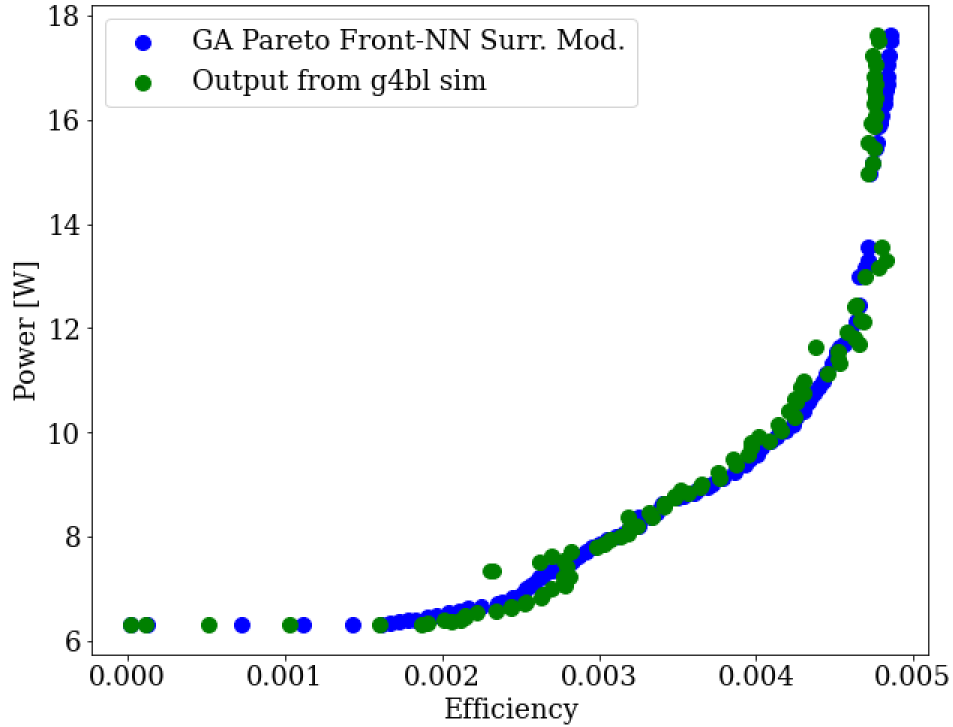
# Genetic Algorithm



# Surrogate model based NSGA-II[1] performance

Optimization to maximize Injection Efficiency/minimize Power Dissipation




- $10^3$ speed up for PCE Surr and $10^4$ speed up for NN Surr
- Agreement within 5% vs 2%  for PCE/NN based GA performance for average injection efficiency of 0.35%

[1] Deb 2002

# Summary

- PSI muEDM experiment will be most precise muon EDM measurement to date → setup needs to be carefully optimized
- Running simulations iteratively is bottleneck in optimization process
- Orders of magnitude speed up can be achieved by replacing physics simulation by surrogate model
- Genetic algorithm NSGA-II used to run multi-objective optimization
- PCE and NN surrogate models based GA investigated; $\sim10^3$ speed up for PCE, $\sim10^4$ for NN
- Plan to expand into Bayesian optimization where higher dimensional input space can be implemented with straightforward uncertainty quantification techniques

# Acknowledgments

The muEDM Collaboration
(Spring meeting 2024)


- Computational resources: PSI Local High Performance Computing cluster, Merlin6, Siyuan-1 cluster supported by the Center for High Performance Computing at Shanghai Jiao Tong University and the Euler cluster operated by the High Performance Computing group at ETH Zürich.
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- NN surrogate starting point: A. Holmberg Bachelor's Thesis ETH Zurich 2021

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# Extra

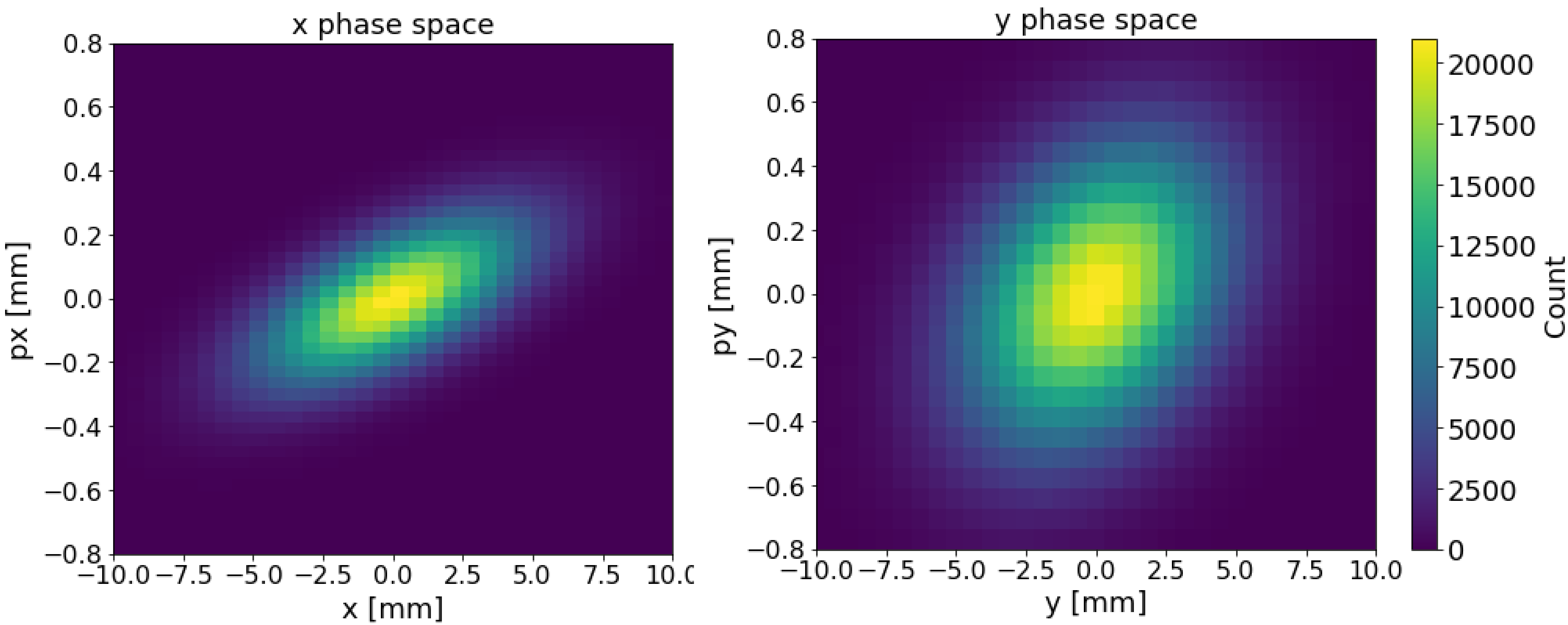
# Polynomial Chaos Orthogonal Basis

*The correspondence of the types of Wiener–Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer).*

| | Random variables $\zeta$ | Wiener–Askey chaos $\{\Phi(\zeta)\}$ | Support |
|---|---|---|---|
| Continuous | Gaussian | Hermite-chaos | $(-\infty, \infty)$ |
| | gamma | Laguerre-chaos | $[0, \infty)$ |
| | beta | Jacobi-chaos | $[a, b]$ |
| | uniform | Legendre-chaos | $[a, b]$ |
| Discrete | Poisson | Charlier-chaos | $\{0, 1, 2, \dots\}$ |
| | binomial | Krawtchouk-chaos | $\{0, 1, \dots, N\}$ |
| | negative binomial | Meixner-chaos | $\{0, 1, 2, \dots\}$ |
| | hypergeometric | Hahn-chaos | $\{0, 1, \dots, N\}$ |

*(Xiu and Karniadakis, 2002)*

# Total phase space after collimation



# Neural Net hyperparameters

```
def __init__(self, input_dimension, output_dimension, n_hidden_layers,
             neurons, regularization_param, regularization_exp):
    super(net, self).__init__()
    # Number of input dimensions n
    self.input_dimension = input_dimension
    # Number of output dimensions m
    self.output_dimension = output_dimension
    # Number of neurons per layer
    self.neurons = neurons
    # Number of hidden layers
    self.n_hidden_layers = n_hidden_layers
    # Activation function
    self.activation = nn.LeakyReLU()
    #
    self.regularization_param = regularization_param
    #
    self.regularization_exp = regularization_exp

    self.input_layer = nn.Linear(self.input_dimension, self.neurons)
    self.hidden_layers = nn.ModuleList([nn.Linear(self.neurons, self.neurons) for _ in range(n_hidden_layers)])
    self.output_layer = nn.Linear(self.neurons, self.output_dimension)

    self.dropout = nn.Dropout(0.1)
```

```
# Model definition
my_network = net(input_dimension=x_train_norm.shape[1], output_dimension=y_train_norm.shape[1],
                 n_hidden_layers=8, neurons=512, regularization_param=0,
                 regularization_exp=0) #2  1e-5


# Random Seed for weight initialization
retrain = 134
# Xavier weight initialization
init_xavier(my_network, retrain)


optimizer_ = optim.Adam(my_network.parameters(), lr=1e-3)#, weight_decay=1e-5)
#optimizer_ = optim.LBFGS(my_network.parameters(), lr=0.1, max_iter=1,
#                         max_eval=50000, tolerance_change=1.0 * np.finfo(float).eps)

scheduler = optim.lr_scheduler.ReduceLROnPlateau(optimizer_, mode='min', factor=0.5, patience=500000)
#scheduler = optim.lr_scheduler.StepLR(optimizer=optimizer_, step_size=50, gamma=0.5)

n_epochs = 200
```

# Neural Net activation function

# 6-d optimization parameter bounds

```
bounds = {"T_Offset": [80, 98],
          "BPI": [0.35,0.80],
          "CC_Len": [88, 150],
          "CC_Ir": [40, 84],
          "CC_Thick":[7,15],
          "CC_Pos":[166,241]}
```