J. Snuverink, M. Frey, C. Baumgarten, A. Adelmann
Paul Scherrer Institut

Precise Modelling and Large Scale Multiobjective Optimization of Cyclotrons

21/11/2019 - FFA2019 PSI
Outline

- Motivation
- New Trimcoil Model in OPAL
- Multi-Objective Optimisation
- Local Search
- Final Results & Conclusions
Obtain Isochronicity in Cyclotrons

- **Uncertainties** in
  - magnetic field (calculation and construction)
  - *injection* parameters ($E_{\text{kin}}, r, p_r,...$)
  - element *positioning* (RF cavities)
  - etc.

- **Restored / Achieved:**
  Additional B-field with *trimcoils* (TCs)
  \[ \Rightarrow \text{phase shift} \]
  (beam gets more/less energy by RF cavities)
  \[ \Rightarrow \text{turn radius shift} \]
Mismatch between Measurements and Simulations

- **Discrepancies / Error in**
  - measured magnetic field due to **measuring conditions, technique and machine accessibility**
  - **simulation model:**
    - discretisation in time and space
    - simplified device models
    - missing device models
    - etc.
  - **injection** parameters ($E_{\text{kin}}, r, p_r, \ldots$)
  - element **positioning** (RF cavities)
  - etc.

Towards quantitative simulations of high power proton cyclotrons.

Mismatch between Measurements and Simulations

- **Discrepancies / Error in**
  - measured magnetic field due to measuring conditions, technique and machine accessibility
  - simulation model:
    - discretisation in time and space
    - simplified device models
    - missing device models
    - etc.
  - injection parameters \( (E_{kin}, r, p_r, ... ) \)
  - element positioning (RF cavities)
  - etc.
Ring tune diagram

Tune diagram for PSI Ring

- Closed Orbit Finder
- Walkinshaw resonance

Energy (MeV)
Ring tune diagram with trim coil 15
New Trimcoil Model in OPAL
Towards More Realistic Trimcoil Simulations

• OPAL PSI-Ring model only contains special TC15

  **but** 18 trim coils in PSI-Ring Cyclotron

• TC-model in OPAL approximated profile with analytical model

  **but** there are TC measurements available

• TC-field contribution in OPAL for 360 degree

  **but** in reality only on sector magnets
New Trimcoil Model in OPAL

• Radial TC profile description with rational function

$$\text{TC}(r) = B_{\text{max}} \frac{\sum_{i=0}^{n} a_i r^i}{\sum_{j=0}^{m} b_j r^j}, \quad n, m \in \mathbb{N}_0 \land r \in [r_{\text{min}}, r_{\text{max}}]$$

tc1: TRIMCOIL, TYPE = "PSI-PHASE",
RMIN = ..., // inner radius [mm]
RMAX = ..., // outer radius [mm]
BMAX = ..., // B-field peak value [T]
COEFS = {a0, a1, a2, a3},
COEFDENOM = {b0, b1, b2, b3, b4, b5};
New Trimcoil Model in OPAL

- **Supported types:**
  - new: PSI-BFIELD, PSI-PHASE
  - old: PSI-BFIELD-MIRRORED

- **Cyclotron-Definition:**

```
Ring: CYCLOTRON, TRIMCOILTHRESHOLD = ..., 
// lower limit of TC contribution [T]
TRIMCOIL = \{tc1, tc2, tc3, ...\}, ...
```
• **Starting point:** Measurement of phase shift effect $\Delta B \sim -\frac{d\Delta \sin(\phi)}{dr}$

---

PSI-Ring Trimcoil Model

• **Fit of phase shift curves:**

\[
\Delta \sin(\phi)(r) \approx h_{\text{phase}}(r) = \frac{f(r)}{g(r)} = \frac{\sum_{i=0}^{n} a_i r^i}{\sum_{j=0}^{m} b_j r^j}
\]

with \( m > n \in \mathbb{N}_0 \)

• **TC2 - TC15:** \( n = 2, \ m = 4 \)

• **TC1, TC16 - TC18:** \( n = 4, \ m = 5 \)

• **Magnetic field:**

\[
B(r) = -\frac{dh_{\text{phase}}}{dr} = -h'_{\text{phase}} = -\frac{f'g - fg'}{g^2}
\]
Multi-Objective Optimisation
Multi-Objective Optimisation (MOO) in OPAL

- **Built-in MOO**:

  \[
  \begin{align*}
  & \text{optimize objectives} \quad f(x) \quad \text{dim}(f) \geq 1 \\
  & \text{subject to constraints} \quad g(x) \geq 0 \quad \text{dim}(g) \geq 0 \\
  & \text{within design variables bounds} \quad x_i^L \leq x_i \leq x_i^U
  \end{align*}
  \]

- **Design variables** \( x \): \( E_{kin}, p_r, \varphi, \text{TC1} - \text{TC16} \) max. B-field, etc.

- **Objectives**: Measure between simulation and real data

  **Note**: \( f \) is our PSI-Ring model + evaluation of objectives!

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Multi-Objective Genetic Algorithm (MOGA)

1st generation

Charles Darwin

Multi-Objective Genetic Algorithm (MOGA)

1st generation

mutation

Charles Darwin

Multi-Objective Genetic Algorithm (MOGA)

1st generation → mutation → crossover

Charles Darwin

Multi-Objective Genetic Algorithm (MOGA)

1st generation

mutation

crossover

2nd generation


Charles Darwin


Multi-Objective Genetic Algorithm (MOGA)

1st generation

mutation

crossover

2nd generation

...
• **Measurements:** Peak intensity of radial profile of probes to distinguish turns

**Figure:** Histogram of RRL measurement
• **Goal:** Match radial peaks of measurement and simulation

• **RRI2:** turns 1 - 16

• **RRL:** turns 9 - 182

190 peaks ⇒ Infeasible number of objectives!

Problem Reduction

• Turn - Aggregation:
  
  • $L_2$-norm

  \[
  \sigma_{[l,u]} = \frac{1}{N} \sqrt{\sum_{i=l}^{u} (r_i^m - r_i^s)^2}
  \]

  • $L_\infty$-norm

  \[
  \sigma_{[l,u]} = \max_{i=l...u} |r_i^m - r_i^s|
  \]

  $N = u - l + 1$: number of aggregated turns

  $r_i^m$: $i$-th turn radii of measurement

  $r_i^s$: $i$-th turn radii of simulation
• **Goal:**
  Find initial injection values

• **Design variables:**
  • beam energy $E_{\text{kin}}$
  • injection angle
  • injection momentum
  • injection radius
  • TC1 - TC4

• **MOO:** (504 cores)
  #generations 500
  #individuals 502

• 5000 particles per individual
• Optimising a few TCs after the other (i.e. optimise sub-problems) leads to divergence! → Optimise full cyclotron at once
• RF cavity voltages not correct → more design variables needed!
• **Single particle tracking** instead of bunch (5000 particles) tracking

⇒ full PSI-Ring simulation in 1 - 2 s

• **Design variables:**
  - injection angle, radius, momentum and energy
  - main cavity voltages
  - phase of Flat-Top cavity
  - voltage of Flat-Top cavity
  - radial position of main cavities
  - radial position of Flat-Top cavity

• **Turn number constraint** to guarantee feasible solutions
Design Variables (48)

1. main RF cavity displacement in radial direction; RF voltage on main cavity 1 - 4
2. displacement of main cavity's axis from global center
3. flat top cavity displacement in radial direction
4. displacement of flat top's axis from global center
5. main cavity's angle w.r.t. the center line of sector magnet 1
6. injection beam energy, injection radial momentum, injection angle of beam, injection radius w.r.t. the global coordinate system
7. positioning of probes (2*3 parameters)
8. flat top cavity angle w.r.t. global coordinate system
9. trim coil maximum magnetic field
10. phase of flat top; RF voltage on flat top cavity
Evolution of best individual during MOGA

>8k individuals/generation

\[ \min_{i=1,\ldots,N} \left( \sum_{j=1}^{M} \sigma_j \right) \text{ [mm]} \]

**Figure:** The label \( \sigma_{[l,u]} \) indicates an objective for the turns in the range \([l, u]\).

\( M \): number of objectives; \( N \): number of individuals per generation.
Result of best individual obtained by MOGA

<table>
<thead>
<tr>
<th>Objective $\sigma[l,u]$</th>
<th>$l_{\infty}$-error (mm)</th>
<th>Probe</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma[1,16]$</td>
<td>6.38</td>
<td>RRI2</td>
</tr>
<tr>
<td>$\sigma[9,31]$</td>
<td>3.76</td>
<td>RRL</td>
</tr>
<tr>
<td>$\sigma[32,61]$</td>
<td>6.34</td>
<td>RRL</td>
</tr>
<tr>
<td>$\sigma[62,105]$</td>
<td>4.39</td>
<td>RRL</td>
</tr>
<tr>
<td>$\sigma[106,148]$</td>
<td>2.91</td>
<td>RRL</td>
</tr>
<tr>
<td>$\sigma[149,182]$</td>
<td>3.27</td>
<td>RRL</td>
</tr>
</tbody>
</table>

**Table:** The label $\sigma[l,u]$ indicates an objective for the turns in the range $[l, u]$. 
Local search after MOGA

• **Issues:**
  - Optimiser suffered with individual selection
  - No further improvements observed
  - Changing many parameters at same time might be disadvantageous

• **Idea:** Local search by simple parameter scanning
  - Often used strategy after genetic algorithm
  - Starting from best MOO individual
  - Change input parameters only in per-mille magnitude
  - Iteratively find worst turn and vary parameters to obtain better individual
    (check $L_\infty$- and $L_2$-norm, $2^{nd}$ and $3^{rd}$ worst turn not to get stuck with only $L_\infty$)
Evolution of maximum absolute error during local search

> 1 mm error reduction after a few iterations
Final Results - RRI2

\[
\Delta r \text{ [mm]}
\]

-6
-4
-2
0
2
4

optimiser local search

turn number

\[
\begin{array}{cccccccccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
\end{array}
\]
Final Results - RRL

-6 -4 -2 0 2 4

$\Delta r \text{ [mm]}$

optimiser local search

turn number

9 19 29 39 49 59 69 79 89 99 109 119 129 139 149 159 169 179

$\Delta r$ [mm]
Wiggly Solution due to TCs - Long Probe RRL1

Optimisation (subset of DVARs) with TCs disabled

Optimisation of above with TCs only
### Final Results

<table>
<thead>
<tr>
<th>Method</th>
<th>$l_\infty$-norm (mm)</th>
<th>MAE (mm)</th>
<th>MSE (mm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>optimiser</td>
<td>6.4</td>
<td>2.0</td>
<td>6.3</td>
</tr>
<tr>
<td>local search</td>
<td>4.5</td>
<td>1.4</td>
<td>3.4</td>
</tr>
</tbody>
</table>

**Table:** Maximum absolute error ($l_\infty$-norm), mean absolute error (MAE) and the mean squared error (MSE) of the best individual of the optimiser and local search compared to the measurement. In both cases the maximum error is at turn 2.
Conclusions

- More realistic generic trimcoil model implemented in OPAL
- Multi-Objective Optimization (MOO) performed to match measurement
  - massively parallel (used with > 1’000 cores)
  - good for finding reasonable solutions fast
  - MOGA possibly not optimal for high-dimensional (> 9) design variable space
  - other algorithms could be considered (e.g. simulated annealing)
- Local search of design variables
  - to improve on MOO solutions
  - may get stuck and stop improving (alternating between metrics helped)
- Realistic model for HIPA Ring cyclotron obtained
  - basis for further studies
- For details please check out Phys. Rev. Accel. Beams 22, 064602 (June 2019)
Wir schaffen Wissen – heute für morgen

Thanks to

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<table>
<thead>
<tr>
<th></th>
<th>$l_\infty$-norm (mm)</th>
<th>MAE (mm)</th>
<th>MSE (mm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>measurement</td>
<td>4.64</td>
<td>1.46</td>
<td>3.59</td>
</tr>
<tr>
<td>space charge</td>
<td>0.05</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

**Table:** Maximum absolute error ($l_\infty$-norm), mean absolute error (MAE) and the mean squared error (MSE) of the measurement or multi particle tracking simulation including space charge to the multi particle tracking simulation neglecting space charge.