Introduction to Intelligent Process Control-Seminar: "what to expect from Al technologies"

IPC-Seminar

Holger Schlarb from DESY Hamburg, 11th of Aug. 2020

Outline:

- Introduction & goal of IPC-seminar ..
- Recap on our accelerators and perspectives
- AI & ML technologies





My background

issues ...

- Studied physics Ffm & HH with some detour on math. (num. PDE/Distr. Theory)
- MSc & PhD in Accelerator Physics in Hamburg (Wakefield comp. / Collimation for TTF)
- 2003 Sabbatical SLAC (SPPS commission)
- 2005 XFEL-WP18 Leader "Special Diag." → 2010 Ch. Gerth
- 2010 XFEL-WP02 Leader "Low Level RF controls" → 2012 J. Branlard
- 2011 Head of "Accelerator Beam Controls" Group (MSK)
- 2017 Involved in DESY's scientific computing strategy discussion



Disclaimer: I am not a computer scientist & not at all in AI !!!!

Studied quite a bit (mainly regarding methodologies / technologies) But: little practical experience Still in learning phase....

Scientific computing @ M-division

What already exists ... & we are pretty strong at

- Numerical codes for beam dynamic simulations...(ASTRA, CSRTrack,...)
- Theory & Simulation of FELs (FAST, Genesis, ALICE)
- Electromagnetic fields simulations (e.g. ECHO) + coop. with TEMF (Darmstadt)
- Fast tracking & opti. codes for operation (RFTweak, OCELOT,...)
- Plasma Wakefield Acceleration (HPC required)





Dedicated Sci. Comp. groups in M-Division (well covered)
 & seminars: e.g. Beam Dynamics XFEL/PETRA/PWA (Igor/Mikheil/Ilya/Max)







Focus of the IPC-seminar:

Why a new seminar?

Intelligent Process Controls...

- ➔ Scientific Computing related to
 - Data mining and data analysis
 - Advanced and data driven controls
 - Fault diagnosis and supervisory control
 - Automated root cause analysis / causal inference
 - Sophisticated automation routines
 - Information extraction technologies
 - Advanced statistical methods and optimization algorithm
 - Explore modern AI methods and technologies

applied to accelerator design, construction, commission and operation



Accelerator & Laser Physics

Interdisciplinary work essential ...

Instrumentation

Both have to learn....

- Control systems
- Infrastructures
- **RF** controls
- . . .

How to interconnect? Sci. Comp. Domain Expert/ize Expert/ize

To be recognized: this is a real challenge!!!

- Information Technologies
- Artificial Intelligence
- Statistics & Math.
- High Performance Comp.
- Control Theory

. . .

Software architecture

- Different language, notation and annotation + pre-existing knowhow ٠
- Different approaches, viewpoints and methodologies •
- limited method overview / adequate implementation / structural analysis / identify use cases **D-Expert:** ٠
- SC-Expert: formulation of goals, system design & interconnect, may own agenda (method) ٠
- Buildup knowhow on the respective other domain (specially language)
- Buildup teams from both domains \rightarrow



Goal of the IPC-seminar:

IPC-seminar should serve

- > Bringing the acc. domain expert and computer science experts together
- > Communication platform for all types of SC problems \rightarrow explore synergies / joint tool development
- > Add tutorial style talks for education and knowledge dissemination
- > Platform to get know to one another (who is working on what with which methods & expertise)
- > Opportunity to present your results or describe your problems
- > Open minded, low barrier ... questions and suggests are welcome ... new field for many of us
- SC@M: concerns M-division as whole / can provide from:
 - Across all accelerator & laser system & test facilities
 - Across M-division groups
 - Currently virtual group in M-division with members in different groups

Intelligent process control of distributed systems

... requires wider expertise ...



Data and computing science – strategy update

First steps towards a DESY wide scienctific computing strategy



Short recap:

DESY's Accelerators & test facilities

DESY accelerators & test benches: birds view ...



VUV & soft-x-ray free-electron laser

Different accelerators ... different challenges

Accelerators at DESY ...



Challenges and degree of matureness very different, but

- → Increased complexity of controls
- → Higher demands on accelerator operations
- \rightarrow Push on the limits regarding performance & flexibility & availability





Beam dynamics of an FEL drive beam

issues ...



Beam dynamics of an FEL drive beam



→ Beam parameters challenging to achieve

Self-Amplified Spontaneous Emission (SASE)

- → Control over 6D phase space mandatory
- \rightarrow kA peak currents causing strong collective effects





L ~ 200m



Wide dynamics range & different operation modes

Time structure & multiple beamline (SA1/SA2/SA3)

- Pulsed operation (RF ~ 1.4ms, 10Hz)
 - → 27000 / sec
 - → e- bunches 220ns spaced
 - 100ms separation
- Bunch distribution & pattern
 - Fast Kicker System
 - Precise (Slow) Flat-Top Kicker
 - 5/10Hz splitting



- Change of beam properties for different beam lines
 - Transients processes
 - Subsystems in different states
 - Large reconfigurations



Challenge: 3 machines in one.... Coupling...





Large and complex Infrastructure & Subsystem

Infrastructure systems (Cryo/Cooling/Power) & large and diverse components ~ 10000 typically



Large number of sensors & components Beam line devices ...



Changes due to digitalization...

Driven by performance requirements and needs for higher flexibility...

Very complex sensor technologies ...





2D detectors / high-speed cameras

DSP



& analog / digital processing units

KALYPSO



MicroProc. \rightarrow DSP's \rightarrow FPGA's \rightarrow SoC \rightarrow MPSoC \rightarrow NoC

Separation from human controls ...



Page 16

What changed over the past decade...

Digitalization changes ...

Classical 3 tier structure + in cooperated Data Acquisition System at EuXFEL



What makes these machine complex ...

Challenge caused by combination of performance / flexibility & availability...

Particle accelerators are ...

- Largely distributed ...
- Various type of systems ...
- Highly non-linear processes ...
- Strongly coupled (sub-)systems ...
- Timing varying disturbances ...
- High dimensionality ~ few 1000
- Use of cutting-edge technologies... (sensors / front-end electronics / real-time processing)
- Limited access to key observables

Facing:

Increasing demand on **Performance**, **Flexibility & Availability**



Future operation & future machines perspectives Questions

- > can we tailored beams with high precision for user experiments
- how far can we push accelerator stability and reproducibility
- > how can we **predict control** over sufficiently long time horizons
- > can we develop **autonomous accelerator** operation
- Can we establish new user-modes to scan the right physics
- > can we build accelerators that predicts failures and repair itself
- > can we **enable new accelerator designs** not accessible today

by applying Advanced Controllers, Data Analytics and AI technologies for *intelligence process control* of accelerators







Artificial Intelligence...

What is artificial intelligence ...

Some definition ...

Artificial intelligence is the attempt to simulate rational or cognitive human intelligence on (technical) machines in order to use it in a profitable and beneficial way for humans @Ralf Otte

Classification:

- 1. Appropriate intelligence adequate reaction to environmental stimuli (I1)
- 2. Learning intelligence independent acquisition of new knowledge (I2)
- 3. Creative intelligence generation of knowledge outside of formal induction and deduction (I3)
- 4. Conscious intelligence Conscious understanding of knowledge (I4)
- 5. Self-confident intelligence conscious understanding of the "ICH" concept (I5)



Example I2: Technical AI systems that are able to apply complex knowledge and at least partially autonomously generate new knowledge

schwache KI

starke KI

- speech processing systems,
- image recognition systems,
- · expert systems,

• ...

- rule-based systems,
- automatic evidence systems,

Remark: Al-definition in Europe (how its done) differs from Anglo-Saxon (what can it do)

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Still

science

fiction

Methodology to gain knowledge

Some definition ...



- Premise (axiom) + inference rules (known knowledge) \rightarrow rules (new knowledge)
- Cause (observed facts) + rules of conclusion (known knowledge) → effect (new facts)

E.g. Statement logic, predicate logic PL1/2, fundamental nature / engineering laws, math. contruction..

Abduction: ("inferring backwards", "applying backwards" a rule base)

• Effect (observed facts) + rules of conclusion (known knowledge) \rightarrow cause (new facts)

Induction: (»learning from data«, creating a non-generally applicable rule base)

• Cause (observed facts) + effect (observed facts) \rightarrow rule (new statistical knowledge)

Remark: in math. <u>full induction is correct</u> since complete!





Al landscape





KI3.0 Induct. + Deduct..

Environment naturell

KI2.0

Induc. + Deduct., Environment quasi

What can you do with data using ML

issues ...



Columns: Variables A....G (called features) Row: set of variable

- Columns: G = f(A,C,E) ask for functional relation (regression) variable to each other?
 → directed relation
- 2. Rows: how many clusters exist?
 → structural analysis
- Individual rows: affiliation to a cluster?
 → structural analysis
- 4. Individual columns to one-another: correlation analysis
 → undirected relation
- 5. Succeeding rows: prediction for following rows
 → trend analysis

ML: first thing you learn ...linear regression...

which is kind of standard for natural scientist & engineers...

Best estimate for
$$\mathbf{y} = \mathbf{f}(\mathbf{x})$$
:
 $w_0 + x_{1,p}w_1 + x_{2,p}w_2 + \dots + x_{N,p}w_N \approx y_p$, $p = 1, \dots, P$.
 $w_0 + x_{1,p}w_1 + x_{2,p}w_2 + \dots + x_{N,p}w_N \approx y_p$, $p = 1, \dots, P$.
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 $w_0 + x_{1,p}w_1 + x_{2,p}w_2 + \dots + x_{N,p}w_N \approx y_p$, $p = 1, \dots, P$.
 $w_0 + x_1w_1 + x_2w_2 + \dots + x_{N,p}w_N = \sum_{p=1}^{p} x_p + \sum_{p = 1}^{p} x_p$

ML: short detour to "Optimization Problems"

most cases finally end up as...

General formulation:

nonlinear program

$$\begin{split} \inf_{z} & f(z) \\ \text{subj. to} & g_{i}(z) \leq 0 \quad \text{for } i = 1, \dots, m \\ & h_{j}(z) = 0 \quad \text{for } j = 1, \dots, p \\ & z \in Z, \end{split} \\ \hline f: \mathbb{R}^{s} \to \mathbb{R}, \ g_{i}: \mathbb{R}^{s} \to \mathbb{R}, \ h_{i}: \mathbb{R}^{s} \to \mathbb{R} \end{split}$$

Cost function Constrains

f,g,h might be

Goal to find z* "the optimizer"

explicit, implicit or as oracles

→ Global optimum $f(z^*) = f^*$



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e.g. polytope for linear inequalities
```

Convex:

 $\lambda z_1 + (1 - \lambda) z_2 \in S \qquad f(\lambda z_1 + (1 - \lambda) z_2) \leq \lambda f(z_1) + (1 - \lambda) f(z_2)$



ML: Nonlinear Feature Engineering...

First steps towards universal approximators...



Represent all possible parameters (weights), also inside fct.

Wavy appears → use trigonometric functions

 $f_1 (\mathbf{x}) = \sin (v_{1,0} + v_{1,1}x_1 + v_{1,2}x_2)$ $f_2 (\mathbf{x}) = \sin (v_{2,0} + v_{2,1}x_1 + v_{2,2}x_2)$

• Elliptical boundaries

model $(\mathbf{x}, \Theta) = w_0 + x_1 w_1 + x_2 w_2 + x_1 x_2 w_3 + x_1^2 w_4 + x_2^2 w_5.$

• Neural network family $f_b(x) = \tanh(w_{b,0} + w_{b,1}x)$







overfitting









ML: clustering methods

... for data structure analysis, outlier identification, ...

Basic sequence of a cluster analysis $U_{n_{SUPervised!}}$ \overrightarrow{DB} Feature
extraction & Cluster
identification
Cluster
identification
Cluster

Classification scheme



→ Likely dedicated talk/tutorial on clustering methods

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Test cases using DBSCAN Density-Based Spatial Clustering of Application with Noise eps=0.4, MinPts=10 und 3.8% Rauschen 6



Artificial neuronal networks as universal approximators

 $w_{0,U_1}^{(1)}$

 $w^{(1)}_{1,U_1}$

÷

Basic intro...

Single neuron: algebraic represented by ٠

$$f^{(1)}(\mathbf{x}) = a \left(w_0^{(1)} + \sum_{n=1}^N w_n^{(1)} x_n \right)$$



1 hidden layers: algebraic represented by ٠

model
$$(\mathbf{x}, \Theta) = w_0 + f_1^{(1)}(\mathbf{x}) w_1 + \dots + f_{U_1}^{(1)}(\mathbf{x}) w_U$$

$$f_{j}^{(1)}(\mathbf{x}) = a \left(w_{0,j}^{(1)} + \sum_{n=1}^{N} w_{n,j}^{(1)} x_{n} \right) \qquad \qquad \mathbf{w}_{1} = \begin{bmatrix} w_{0,1}^{(1)} & w_{0,2}^{(1)} & \cdots & w_{0,U_{1}}^{(1)} \\ w_{1,1}^{(1)} & w_{1,2}^{(1)} & \cdots & w_{1,U_{1}}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ w_{N1}^{(1)} & w_{N2}^{(1)} & \cdots & w_{NU_{1}}^{(1)} \end{bmatrix}$$



model

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 X_1

New feature

(sub-symbolic)

0

0

Artificial neuronal networks as universal approximators

Basic intro...

Multi-layer neural networks:

model (\mathbf{x}, Θ) = $\mathbf{w}_{L+1}^T \mathbf{a} \left(\mathbf{W}_L^T \mathbf{a} \left(\mathbf{W}_{L-1}^T \mathbf{a} \left(\cdots \mathbf{a} \left(\mathbf{W}_1^T \mathbf{x} \right) \right) \right) \right)$

→ concatenated chain of multi-dim. function

- \rightarrow allows to approx. arbitrary functions
- Specialties of ANNs
 - Structure: parallel distributed processing
 - Natural propensity for storing experiential knowledge
- Break through:
 - Efficient training methods (initialization, regulation techniques, batch-training, dropout, efficient optimizers, avail. libraries....)
 - GPUs: massive improvement on parallel processing
 - Remark: large ANN still takes a long time to train
- ANN strength: Enhancement due manipulation of sub-symbolic elements
- ANN criticism: Missing interpretability of sub-symbolic elements





Example full-connected neural network for two-class dataset

Some special types of ANN:

kernel K

Basic intro...

- Convolutional NN:
 - Mainly of image processing
 - Feature maps using convolution



$$K[i, j] = (K * I)[j, j] = \sum_{m} \sum_{n} I[i + m, j + n] \cdot K[m, n]$$

Typically 3x3 / .../11x11



- Specialty:
 - learns kernel function for feature maps
 - Sparse interactions
 - Parameter sharing
 - Equivalent representations

96 kernels 11 x 11 first layer feature map (60M param/650k Neur.)



Ref: Hinten2017 DOI:10.1145/3065386

Some special types of ANN:

Basic intro...

- Autoencoder-NN:
 - For feature reduction / extraction.
 - Target value is input value y = x
 - Ask for a function of type

 $x = f_{dec} (f_{enc}(x))$

- Specialty:
 - Use for data reduction
 - Noise removal
 - Non-linear dimension reduction
 - Decoupling of learning cycles (weak hardware)





Some special types of ANN:

Basic intro...

- TM-Polynomial-NN:
 - Activation functions are polynomials
 - E.g. solving non-linear ordinary differential equations

$$\frac{d}{dt}\mathbf{X} = \mathbf{F}(t,\mathbf{X}) = \sum_{k=0}^{\infty} P^{1k}(t)\mathbf{X}^{[k]}, \text{ F as Taylor expansion}$$

- Evolution of system from $t_0 \rightarrow t$ expressed by Matrix Lie maps

$$\mathbf{X}_{i+1} = \mathcal{M} \circ \mathbf{X}_i = W_0 + W_1 \begin{pmatrix} x_i \\ y_i \end{pmatrix} + W_2 \begin{pmatrix} x_i^2 \\ x_i y_i \\ y_i^2 \end{pmatrix} + W_3 \begin{pmatrix} x_i^3 \\ x_i^2 y_i \\ x_i y_i^2 \\ y_i^3 \end{pmatrix}$$

- 1) ODE \rightarrow calc. W \rightarrow efficient numerical solver for ODL
- 2) Trajectory \rightarrow train W \rightarrow extract ODL
- Specialty:
 - Shallow but very deep nets
 - Clear interpretation of weights
 - Trick: Regularization includes symplecticity of W_i

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typical architectures





→ Talk by Andrei Ivanov

To wrap up

- Digitalization and complexity increase of accelerator → new tools for controls required
- Supervisory control of processes mostly requires to build models of your systems:

DeductiveInductive or
IdentificationInductive or
Black boxJust from data
$$\leftarrow$$
 Excite systemGrey boxDeductive &
InductiveModel y = f(x), but
often x = f^1(y) required

- AI & ML (I2): allows to construct models / rules from data, but they are of statistical nature
- Strength of ANN: learning and manipulation of sub-symbolic elements derived from features
- Data Mining: make use of our data base for better understanding of our systems on all levels
- **Predictive controls:** we like to achieve \rightarrow prediction of accelerator behavior for finite time horizons
- Goal of seminar: bring to together the various domain experts across M-division

Some additional information

 Machine Learning at DESY: <u>desy-ml@desy.de</u> Indico page: <u>https://indico.desy.de</u>

https://indico.desy.de/indico/category/641/

- OWLE: Virtual seminar series on computational accelerator physics, machine learning and experimental demonstration of AI-ML; https://sites.google.com/view/owle/
- IPC mailing list: <u>ipc-info@desy.de</u>
- IPC confluence: <u>https://confluence.desy.de/display/IPC</u>
 - IPC seminar: https://indico.desy.de/indico/category/740/

October 2020

20 Oct Sergey Tomin, "OCELOT" (New!

September 2020

- 22 Sep Gianluca Valentino, "Reinforcement Learning applications in particle accelerators"
- 08 Sep Maxence Thevenet, "Introduction to High Performance Computing"

August 2020

25 Aug Prof. Gerwald Lichtenberg, "Automated Fault Detection and Diagnosis - an Introduction"



General Contact:

- Annika Eichler
- Raimund Kammering
- Ilya Agapov
- Holger Schlarb

Thanks for attention

Literature:





Francesco Borrelli Alberto Bemporad

Aanfred Morari

ISBN 978-1-491962299



Quantum Computing

verstehen



ISBN: 978-3-527-71494-0



And many more....



ISBN 978-1-85233-694-3

Reinforcement Learning Algorithms with Python



ISBN 978-1-789-111-6