Thoughts for Dynamic Systems:

How A Better Model Can Help Us Understand and Control Intelligently

Sandra Gail Biedron, Ph.D.

Element Aero

And

Electrical and Computer Engineering and Mechanical Engineering, the University of New Mexico

On behalf of many collaborators *and others sending us inspiration and support*

LEAPS Integrated Platform Workshop
11-12 May, 2021

Thank you

- Thank you for the invite. *This was a great forum in which to gather back with my many long-time colleagues. Wish only we were in person……*
- Today I want to focus in a few minutes on a few ideas and examples in the requested "teaser talk".
- Taking heavily from my talk recently at ORNL's Artificial Intelligence for Robust Engineering & Science (second in the series - AIRES 2: MACHINE LEARNING FOR ROBUST DIGITAL TWINS), January 19-21, 2021 AIRES

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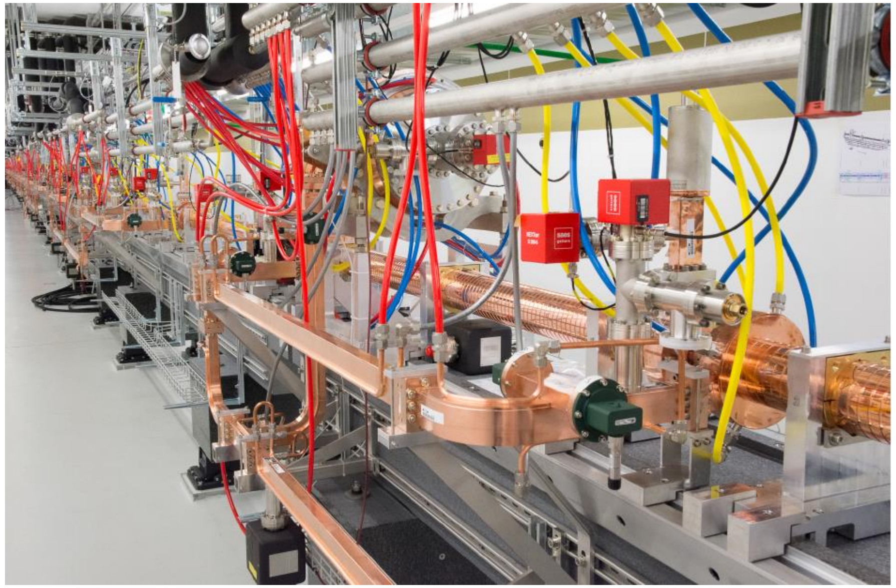
Collaborators

UNM – **Sandra Biedron, Manel Martinez-Ramon**, Steve Conradson, Trudy Bolin, Mariana Fazio, Sal Sosa, Aasma Aslam, Destry Monk, Jorge Alberto Diaz Cruz, Shannon Scott, Reza Pirayesh, TJ Schaub
Argonne - Michael Papka and David Martin
BNL – Marcus Babzien, **Kevin Brown, Mark Palmer**, Bob Malone, Jing Tao, Mikhail Fedurin, Junjie Li
LANL – **Alan Hurd,** John Sarrao, Christine Sweeney, Evgenya Simakov, John Lewellen, Nathan Moody, Stephen Milton, Julian Chen, Rohit Prasankumar, Toni Taylor
USC – Clio Gonzalez-Zacarias
Stony Brook – Bohong Huang, Thomas Robertazzi
Space Dynamics Laboratory – Asal Naseri
New Mexico State University, - Steven Stochaj
NASA Goddard Space Flight Center – Neerav Shah
NASA Universities Space Research Association – John Krizmanic
JLAB – Shukui Zhang
Element Aero – Dave Caulton
ILS – Mark Curtin
FRIB – Steve Lidia
UCLA – Jamie Rosenzweig

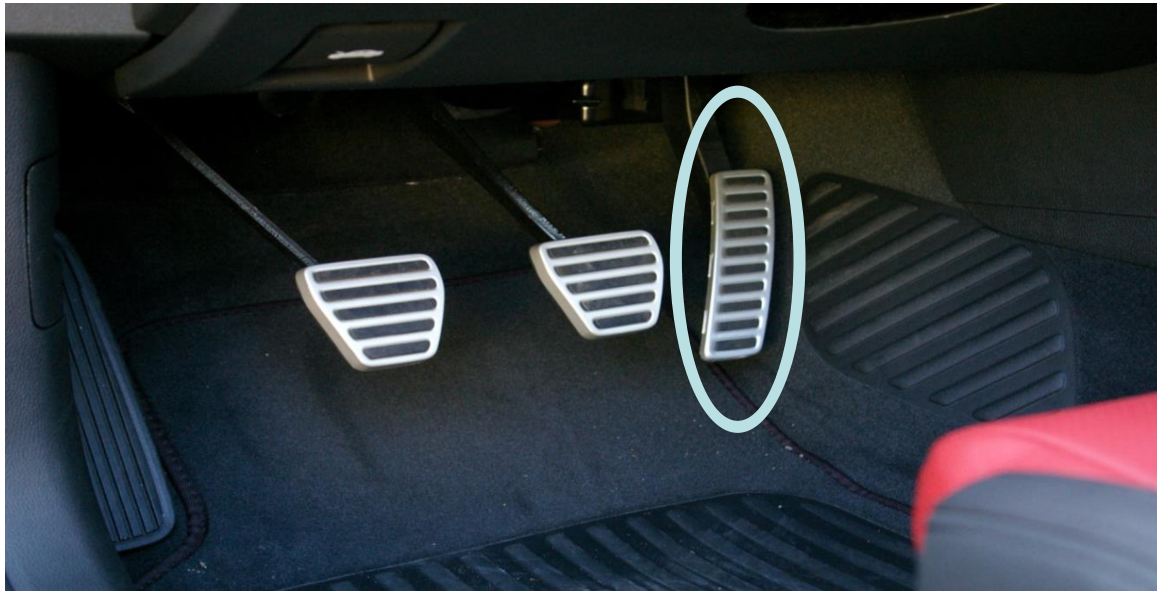
and inspiration of many others!

How I got here (HERE = Data science)
*Confessions of an accelerator physicist***

- And no, I do not mean a car's accelerator ***in reference to self-driving cars***
- ***And since my buddy from GM is not here, I can pick on self-driving cars.***



My vision of a research infrastructure – an ***accelerator*** with particles traveling close to c (Swiss FEL)



GM's Dave Brooks' vision of an ***accelerator***
With top speed of ~130 km/hr

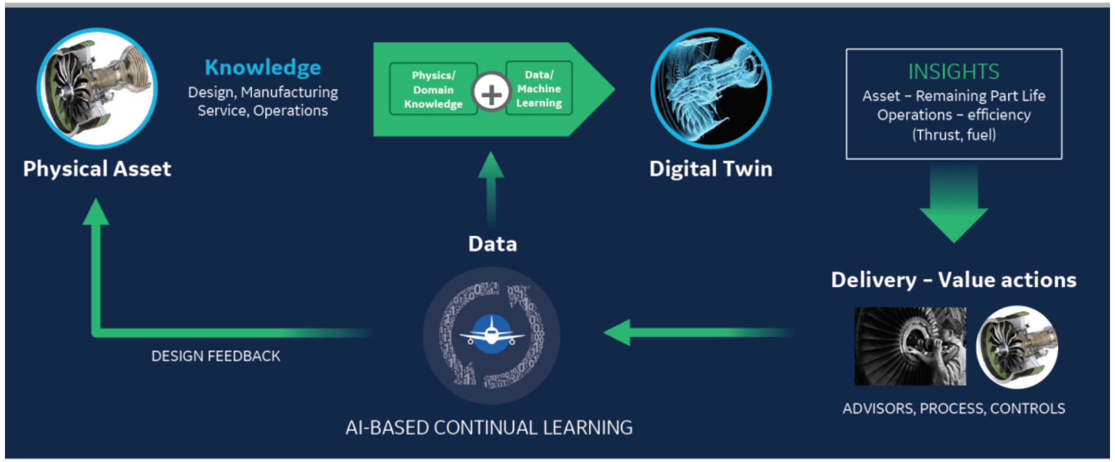
I just "…want to go fast…" for 2000+ user hours per year, without jitter, with a constant beam size and charge, without accidental shut down, rapid user-driven changes etc. ***Much can be said of all scientific research infrastructures.*** ***How can digital twins help us make research infrastructures better?***

**With a *minor* obsession about control and use of aircraft, including aircraft/aerial platforms for defense and security.

Real/Digital twins – industry and science

- **Industry Example**
  - Can be that there are many improvements as there are more physical replicas (*e.g. digital twin aggregates)*
  - Can be that there is an update to the manufacturing process

Extracting value: Digital Twin | A personalized, living, learning, model



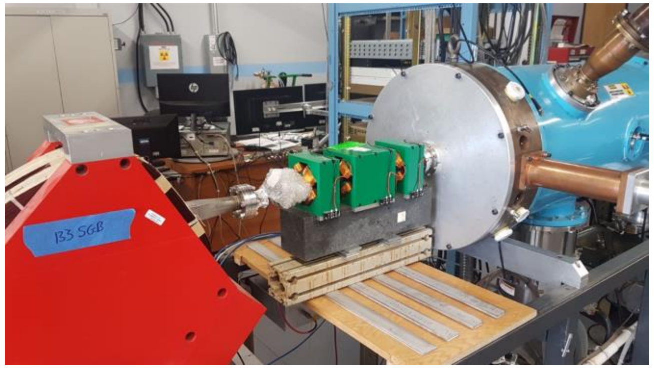
CONTINUOUSLY IMPROVING BUSINESS OUTCOMES

Example from Colin Parris, Vice President, Software and Analytics Research, GE Research, DOE AI InnovationXLab Artificial Intelligence Summit, October 2019, Chicago, Illinois

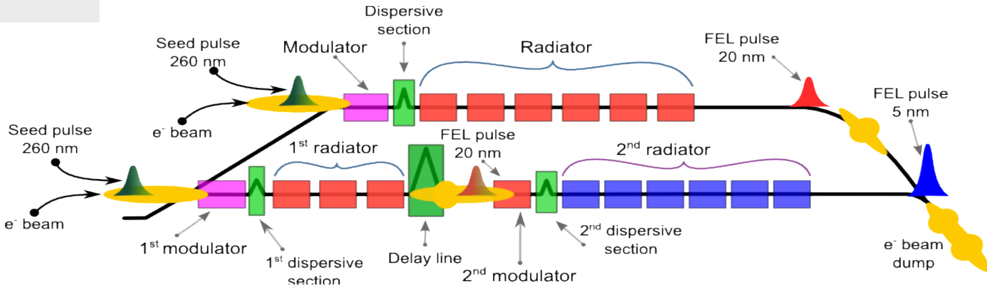
- **Research Infrastructures Example**
  - Many times these are "one offs" (DTI)
    - Satellites and Spacecraft
    - Particle Accelerators
    - Lasers
    - Quantum Computers
    - Etc.

IBM and Goppion Collaboration

L3 HAPLS (The High-Repetition-Rate Advanced Petawatt Laser System) at the Extreme Light Infrastructure Beamlines



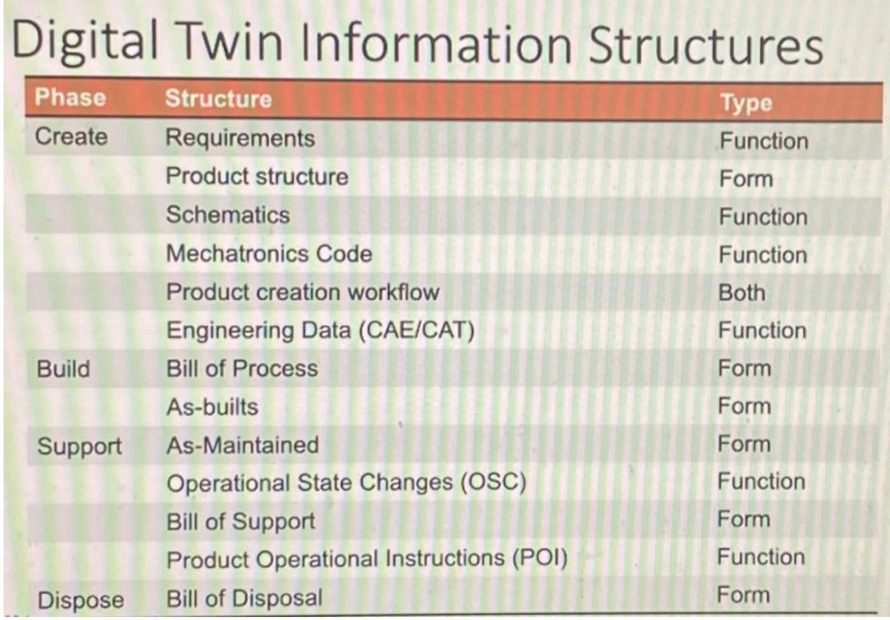
Ion Linac Systems Medical Accelerators



Echoing Michael Grieves – DT Prototypes, Instance, Aggregates

Fermi@Elettra User Facility

Other thoughts

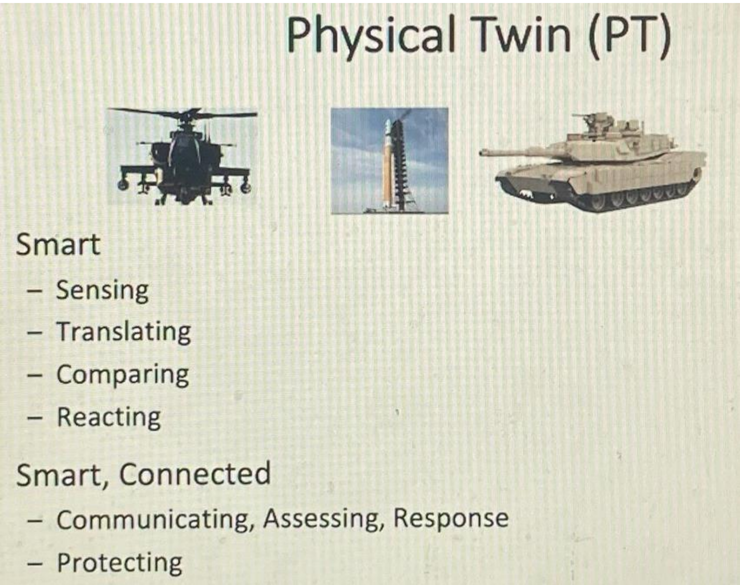


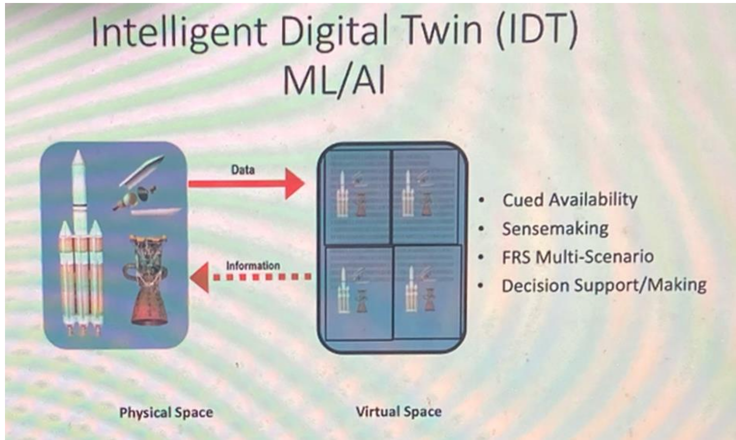
Digital Twin Information Structures

Phase	Structure	Type
Create	Requirements	Function
	Product structure	Form
	Schematics	Function
	Mechatronics Code	Function
	Product creation workflow	Both
	Engineering Data (CAE/CAT)	Function
Build	Bill of Process	Form
	As-builts	Form
Support	As-Maintained	Form
	Operational State Changes (OSC)	Function
	Bill of Support	Form
	Product Operational Instructions (POI)	Function
Dispose	Bill of Disposal	Form

- Digital Twin Types
  - Digital Twin Prototype
    - All that CAN BE made
  - Digital Twin Instance
    - All that ARE made
  - Digital Twin Aggregate
    - Identically made

Fallacy:
a digital twin requires a physical counterpart





Models

- Models of systems can help provide insight into the dependencies and interfaces between the various subsystems.
- Having worked on defense and industrial projects since the very beginning of my career, I apply approaches such as ***model-based systems engineering. The "model" is increasingly important and is not steady state, which plays into controls (that plays into the models - combining physics and data driven - being on the edge and on HPCs)***

Models based systems engineering

- In systems engineering practices, ***models reign***.
  - One definition - **"Model-Based Engineering (MBE): An approach to engineering that uses models as an integral part of the technical baseline that includes the requirements, analysis, design, implementation, and verification of a capability, system, and/or product throughout the acquisition life cycle."** (Source Final Report, Model-Based Engineering Subcommittee, National Defense Industrial Association, Feb. 2011).
  - This definition does not entirely capture the model being used after a system is delivered but the model can be used later – like being updated constantly for refining the understanding of the system and being used to monitor its health as well as controlling it.

All systems work together – Something always said in Physiology but not often in SE

INCOSE MBSE Initiative - https://www.incose.org/incose-member-resources/working-groups/transformational/mbse-initiative

Models based systems engineering

- We saw and continue to see clearly in several industry and defense cases that a more comprehensive model was/is needed that could help better design and understand the system *as well as for health monitoring of the system and control the system* out to the use case.
- Data science helps build off of our first principles models, help systems that might not have first principles models, and help understand systems that might not have much experimental data, etc.

"All models are wrong, but some are useful" George E. P. Box

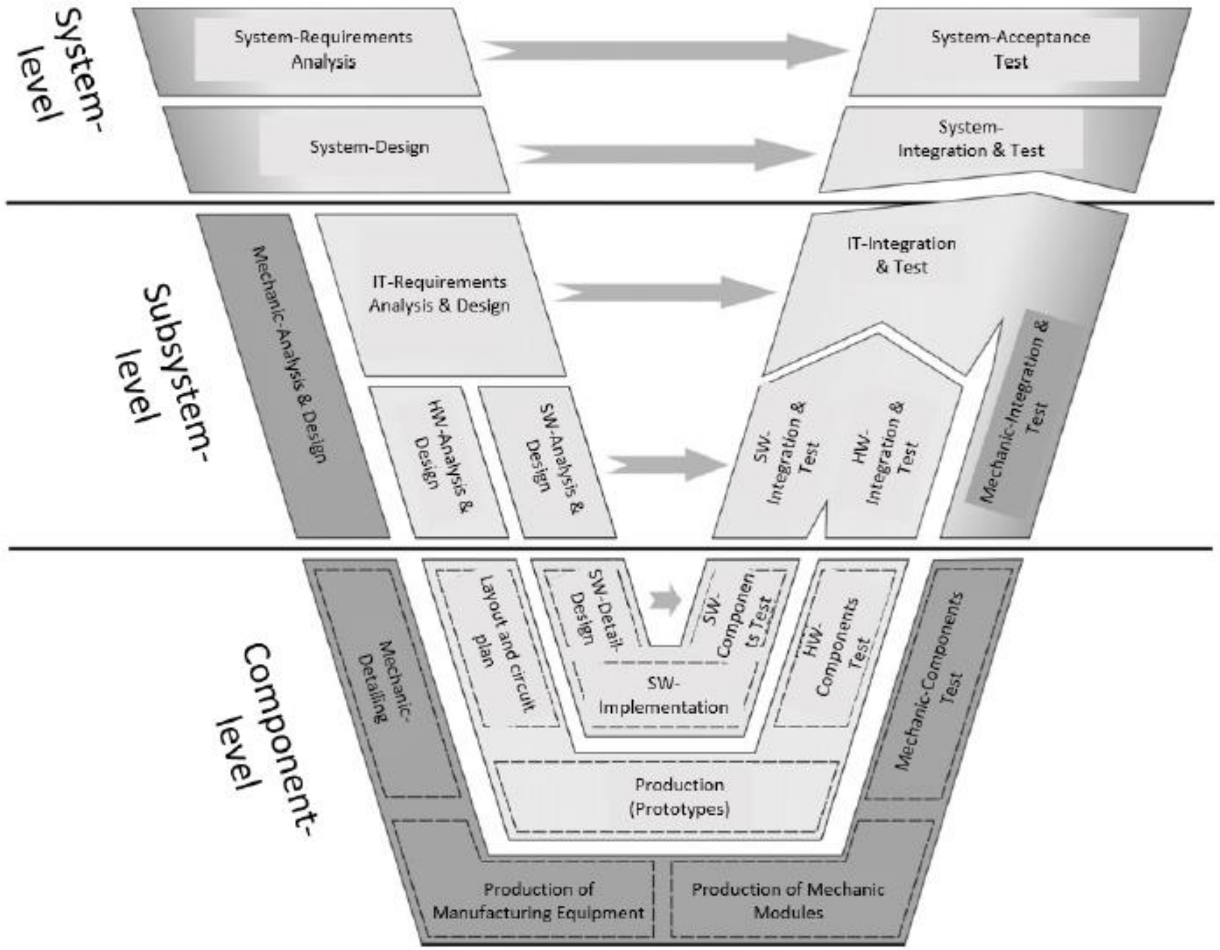
but we can to our best try to build the best model possible

Models based systems engineering

Requirements DEFINE our systems but also the data intensive/driven sub-systems *part of the systems engineering design process*

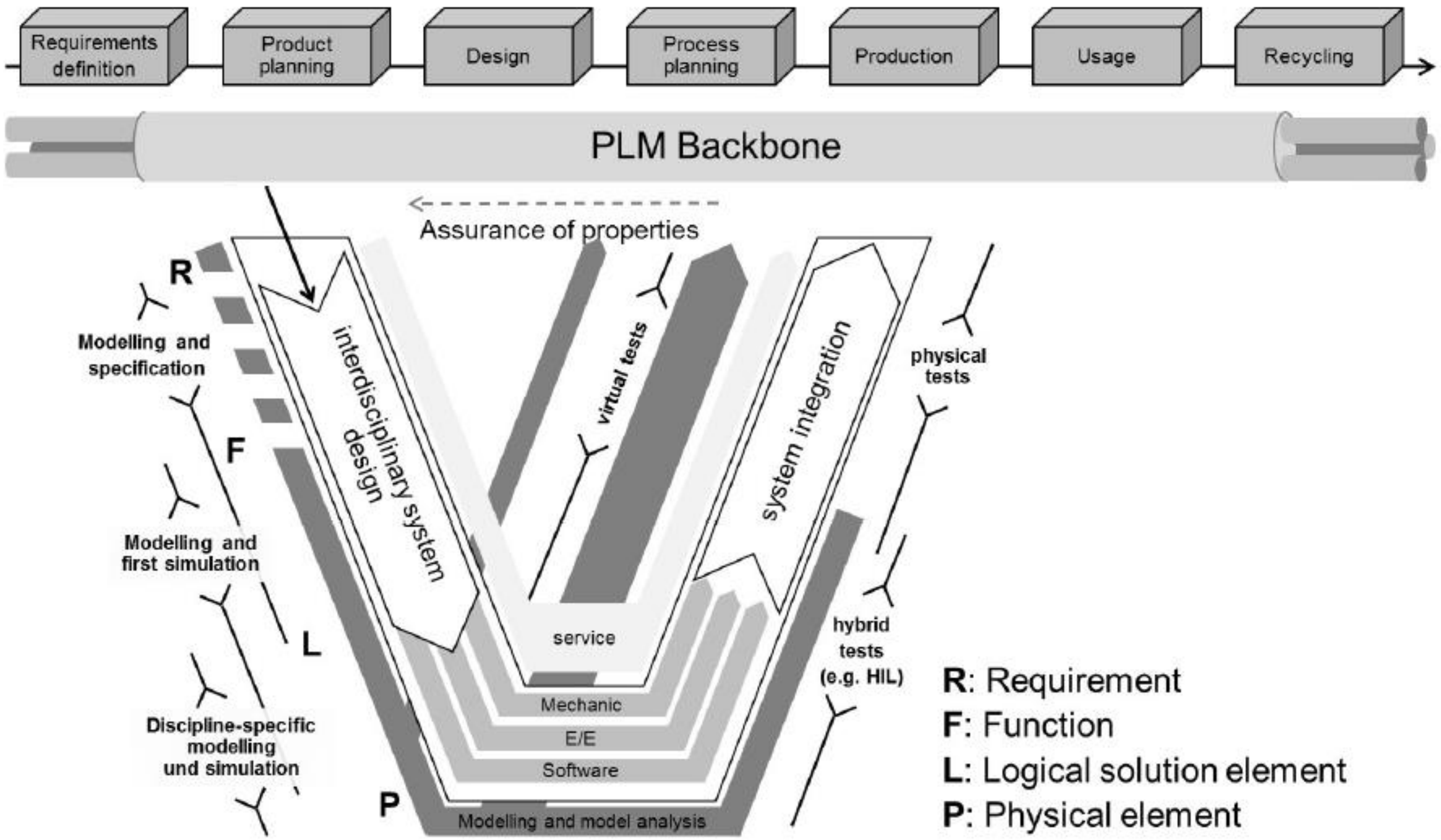
- To what level do you want definition in a to be built system? Reflect this in the digital model. *For instance, if you intend to control it well, are your controllers part of your model/twin?*
- Is there a requirement driving an ML/AI component of your system?
- For the sub-system of computing/data science (e.g. ML/AI), storage, and sensors, do you have enough power, bandwidth?
- First principles/simulated physics (with anchored codes), physics informed, and mathematical programming important. Reduce computation.
- While models are build up – all domains have to be considered simultaneously.
- How much data is enough for on-line modeling? How much data is enough in terms of storage (what do we keep/throw out)?
- Do you need more sensors? Do you have the right sensors? What is a sensor breaks? Are we sampling at the right rate to give us the data on the correct time scales for the given device/sub-system for things like prognostics? Etc.
- The AI/ML techniques also might need to be updated as more data is collected and contributed to a learned model. So in fact, the systems engineering for the data backbone might not be steady state.
- Updating the physics over time as a function of use, *e.g. materials in nuclear reactors failing*.
- How do you know when you are done?

V diagram examples



Bender, K. (2005), Embedded Systems - qualitätsorientierte Entwicklung, Springer-Verlag, Berlin,Heidelberg. https://doi.org/10.1007/b138984

V diagram examples



Extended V-model for model-based systems engineering (Eigner et al., 2012)

Eigner, M., Gilz, T. and Zafirov, R. (2012), Interdisziplinäre Produktentwicklung - Modellbasiertes Systems Engineering. [online] PLM portal. Available at: https://www.plmportal.org/de/forschungdetail/ interdisziplinaere-produktentwicklung-modellbasiertes-systems-engineering.html (accessed 12.03.2018).
Eigner, M., Koch, W. and Muggeo, C. (2017), Modellbasierter Entwicklungsprozess cybertronischer Systeme: Der PLM-unterstützte Referenzentwicklungsprozess für Produkte und Produktionssysteme, Springer Vieweg, Berlin, Heidelberg. https://doi.org/10.1007/978-3-662-55124-0

Let's look at a few examples

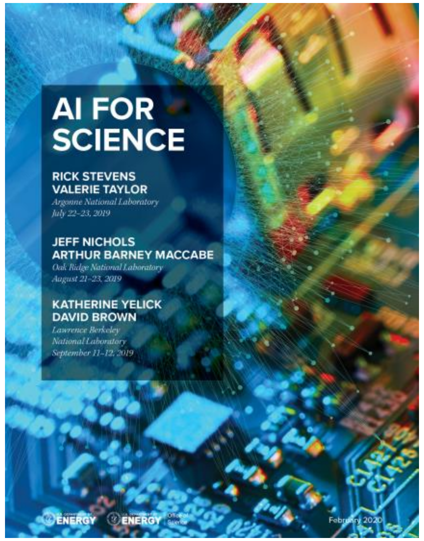
- Satellite-based telescope
- Quantum Information Science System
- C-Band Compact X-Ray Free-Electron Laser
- Materials Discovery
- Imaging

"Digital twins" reference transformational approaches for expanding optimization to include an entire manufacturing lifespan, from raw materials to shape/topology to manufacturing process to end use

- Can perform information fusion from disparate sources
- Coupling real-time data with models (e.g., a "digital twin")
- AI-driven, real-time intelligence
- Surrogate models could form the basis for digital twins that guide design and operation.

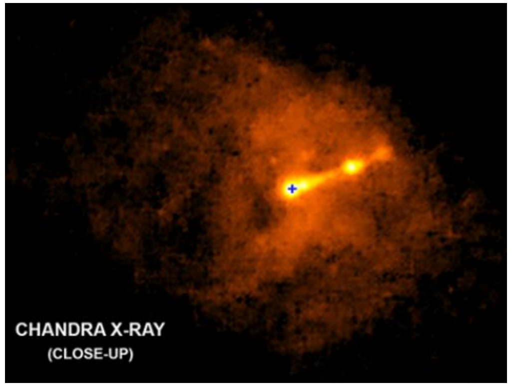
Report on the Department of Energy (DOE) Town Halls on Artificial Intelligence (AI) for Science, February 2020

The combination of machine hardware, advanced computing for simulation, and data science for surrogate modelling, training of neural networks and data analysis is inspired by our past work and our participation on DOE meetings, workshops and reports such as AI for Science (*https://www.anl.gov/ai-for-science-report*).

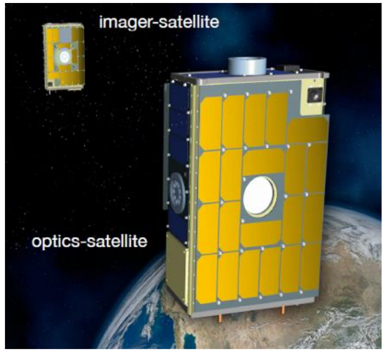


Satellite-based telescope

- Data-based machine learning control system for the Virtual Telescope for X-ray Observations (VTXO)
- Applications
  - Investigating the nature of space
  - Understanding more about black holes
  - Exploring the Sun
  - Detecting space phenomena: An example is detection of the stars' collision
  - Finding extraterrestrial life



Satellite-based telescope

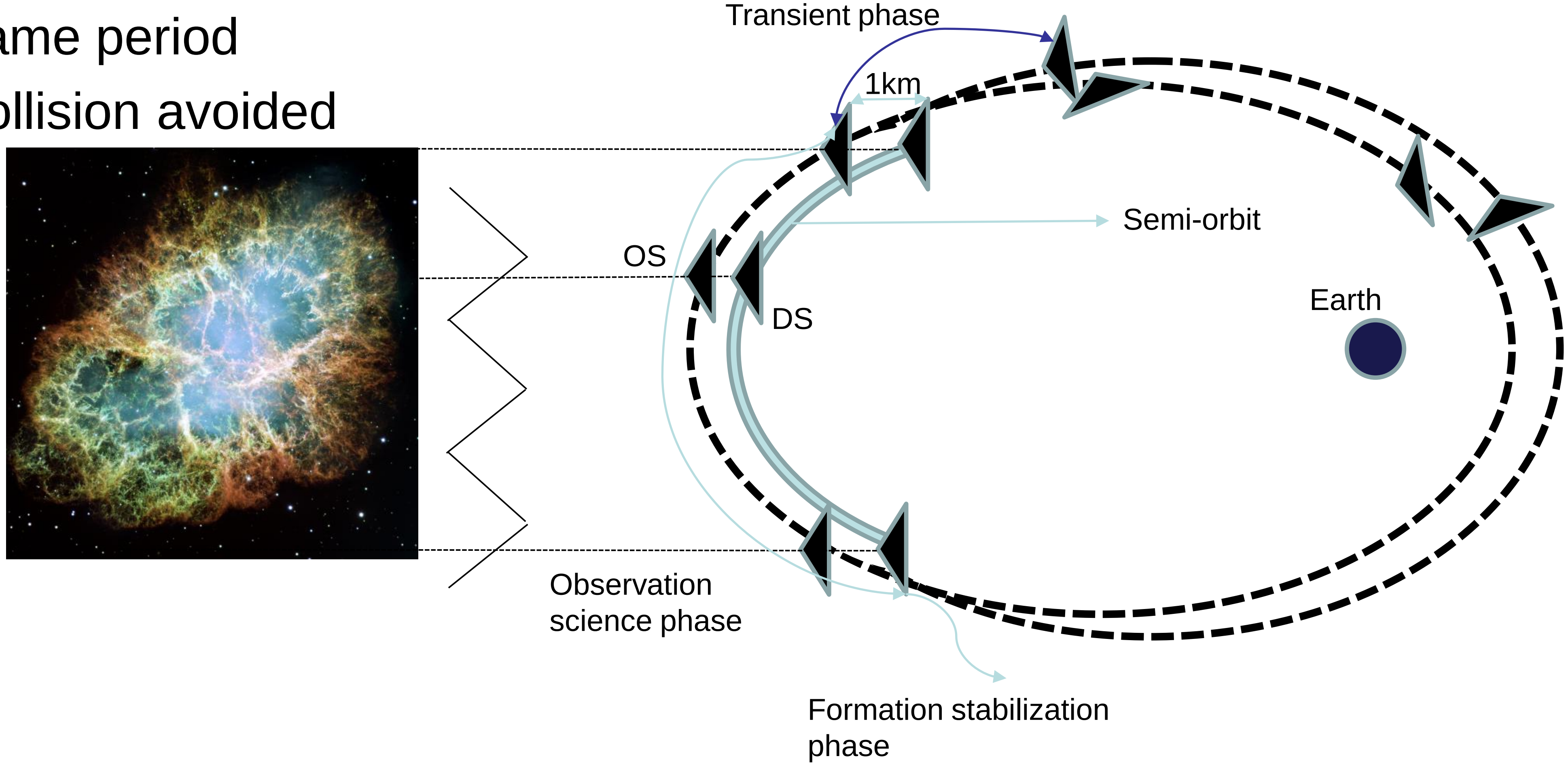


Requirements

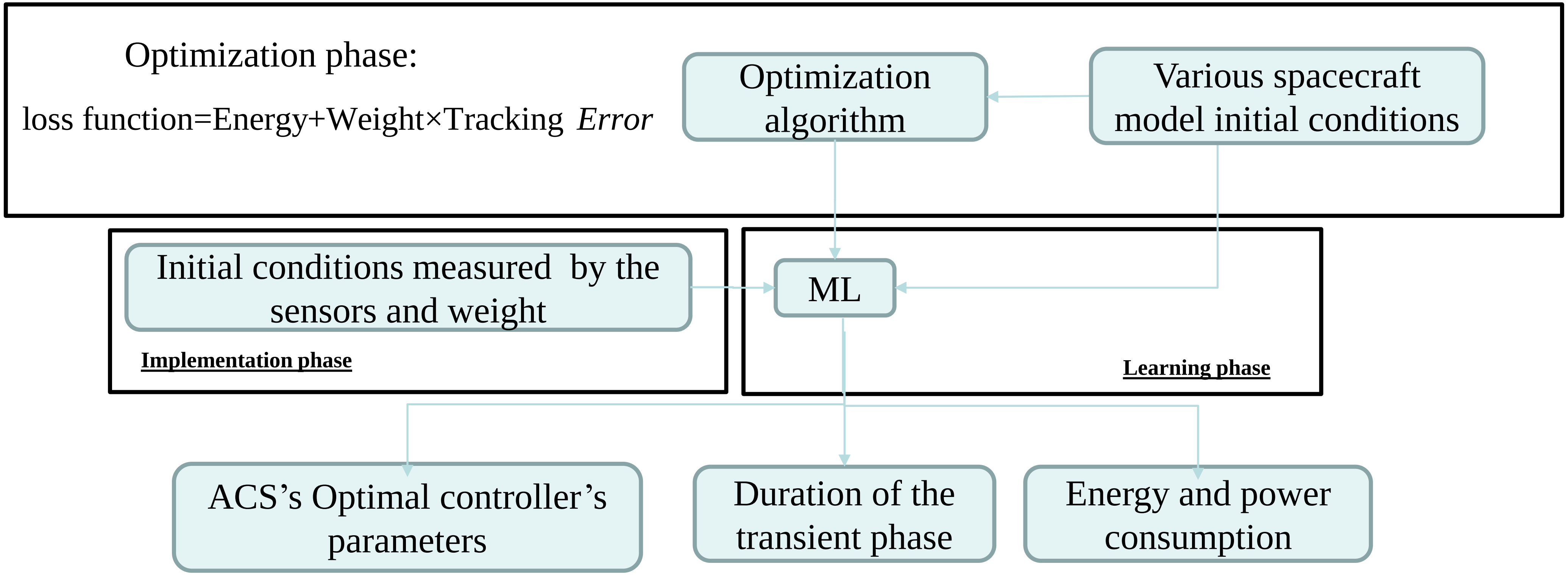
- Telescope for virtual for x-ray observations
- Attitude formation control with sub-arcsecond accuracy
- Highly eccentric geostationary orbit
- Approximately 16 hours observing the Crab Nebula
- Distance between the imager-satellite and optics-satellite is 1 km
- We are relying on and helping to improving upon a model of the overall system based on our “sub-model” for control of the system.

Satellite-based telescope

- The orbits have the same parameters except the eccentricity
- Same period
- Collision avoided



Satellite-based telescope



Reza Pirayesh, Jorge Diaz Cruz, Sandra Biedron, Manel Martinez-Ramon, Salvador Sosa, Asal Naseri, "Intelligent real-time robust nonlinear attitude control for Virtual Telescope for X-ray observation," manuscript in preparation for IEEE Access.

Satellite-based telescope

- The nonlinear Lyapunov controller is robust against system uncertainty.
- To reach the desired sub-arcsecond accuracy, we introduce additional constraints and techniques, such as relative position, more sensors, image processing techniques, filtering techniques, reinforcement learning, and at the end the system still need to be modeled as a complex hybrid intelligent system.

Reza Pirayesh, Jorge Diaz Cruz, Sandra Biedron, Manel Martinez-Ramon, Salvador Sosa, Asal Naseri, “Intelligent real-time robust nonlinear attitude control for Virtual Telescope for X-ray observation,” manuscript in preparation for IEEE Access.

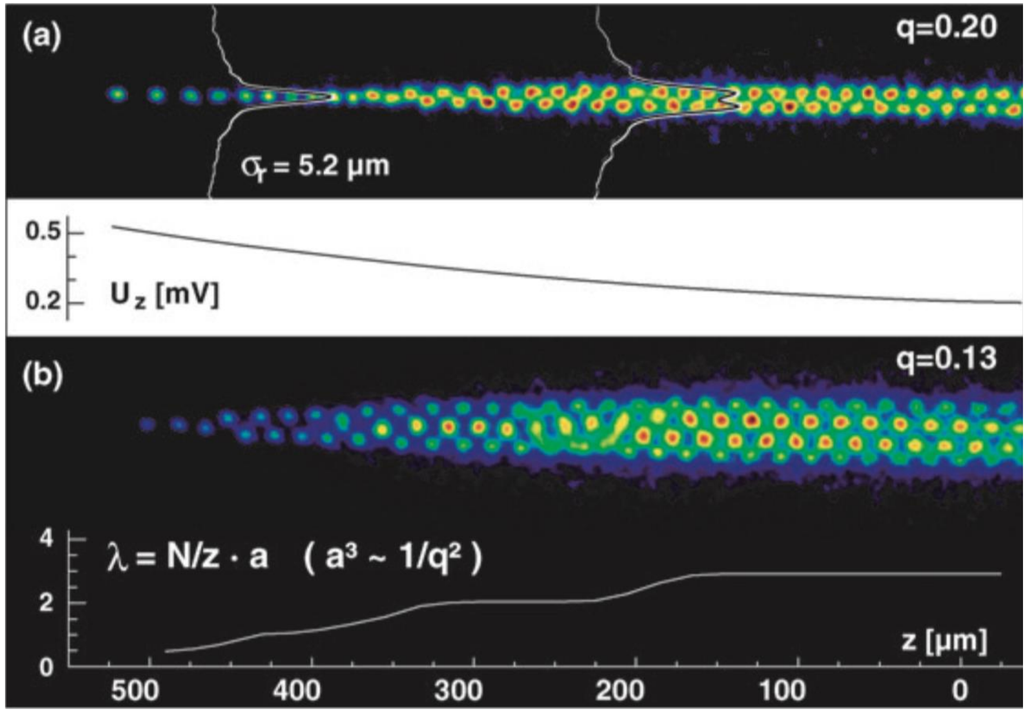
Satellite-based telescope

- Simulated annealing for producing data with the loss function
- Grid search and randomized search for optimizing the hyperparameter with mean absolute percentage error (MAPE) and mean square error (MSE)

Reza Pirayesh, Jorge Diaz Cruz, Sandra Biedron, Manel Martinez-Ramon, Salvador Sosa, Asal Naseri, “Intelligent real-time robust nonlinear attitude control for Virtual Telescope for X-ray observation,” manuscript in preparation for IEEE Access.

Use of Ion Coulomb Crystals in Storage Rings for QIS

- **Ion Coulomb crystals (ICC) - chains of ions**
  - cooled below the Doppler limit, but not to the point of the Lamb-Dicke limit (i.e., to the resolved sideband limit)
  - True quantum systems - not simulations
- **Exploit two quantum properties**
  - external eigenstates (quantum phonon modes)
  - internal eigenstates (hyperfine spin states)
- **Decoherence?**
  - quantum states in trapped ions can persist for very long times (>hour)
- **Entanglement - Yes.**
  - exploit the coupling of the internal and external quantum states of the ions
- **Will go beyond Noisy Intermediate-Scale Quantum (NISQ) systems**
  - Quantum computation with error correction can be implemented
- **Classical Control & Computing support for massive scale QIS**
  - How to efficiently scale up - needs R&D



U Schramm, T Schätz, M Bussmann and D Habs Plasma Phys. Control. Fusion **44** (2002) B375–B387

Kevin Brown and Thomas Roser of BNL SRQC concept

Use of Ion Coulomb Crystals in Storage Rings for QIS

Being Provocative

- In a single volume: as many as 100,000 ions/revolution
- In a single volume we can create multiple long ICCs
- Imagine 100 ion long ICCs. A single volume could contain hundreds.
- For comparison, modern ion traps can contain 20-200 ions/trap
- Having constant velocity enables time-of-flight methods of selecting different ions in the crystal (every ion can be tagged)
- From the same ring could run multiple & separate quantum computations
- ICCs can be used as memory as well as for error correction algorithms
- High degree of parallelism - multiple lasers, etc.

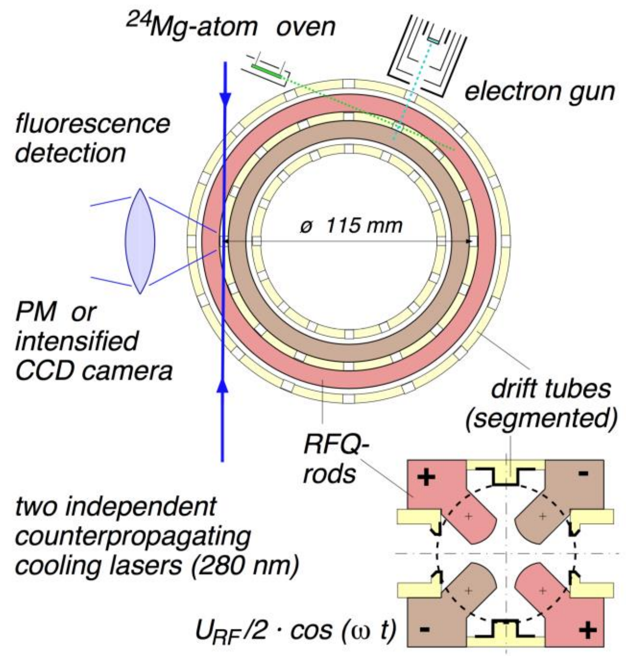
PHYSICAL REVIEW ACCELERATORS AND BEAMS **23,** 054701 (2020)

Towards storage rings as quantum computers

K. A. Brown* and T. Roser
Brookhaven National Laboratory, Upton, New York 11973-5000, USA

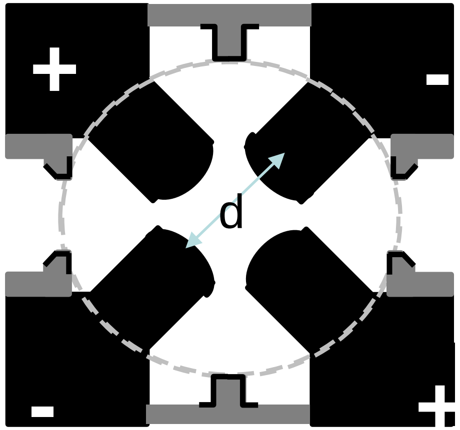
(Received 28 February 2020; accepted 4 May 2020; published 13 May 2020)

We explore the possible use of particle beam storage rings as quantum computers. More precisely, we consider creating an ion trap system, in which the same computational basis states can be defined as in a modern ion trap system, but in which the ions have a constant velocity and are rotating in a circular trap. The basic structures that we explore are classical and ultracold crystalline beams. What we propose is a novel method that uses the ion trap quantum computer concept, but puts the ions into a rotating frame of reference. The benefits of this approach are discussed.



U Schramm[1], T Schätz, M Bussmann and D Habs

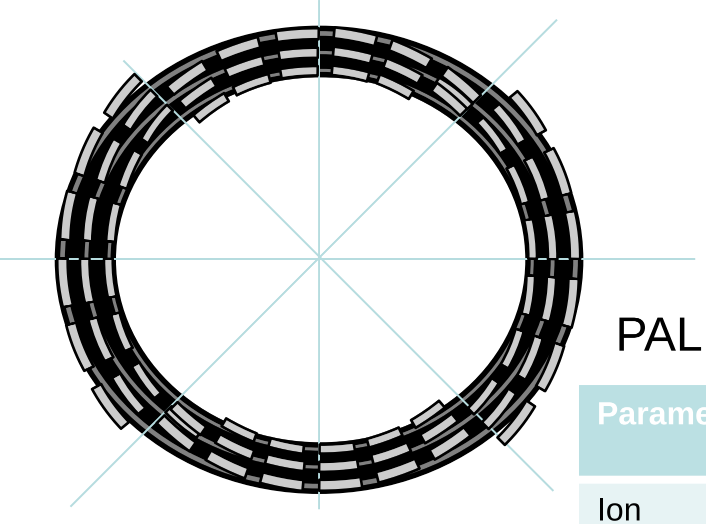
Design of the Storage Ring QC



Parameter	Value	Units/notes
Conducting Rings	Titanium	Coef. Exp 9.4×10^{-6}/K
Supporting Rings	Ceramic	
Drift tubes	Gold	
d	5	[mm]
Ceramic coef. Exp.	6.9×10^{-6}	[1/K]
Vacuum	$<10^{-11}$	kPa ($\sim 10^{-10}$ Torr)
Drift gap	~2	[mm]

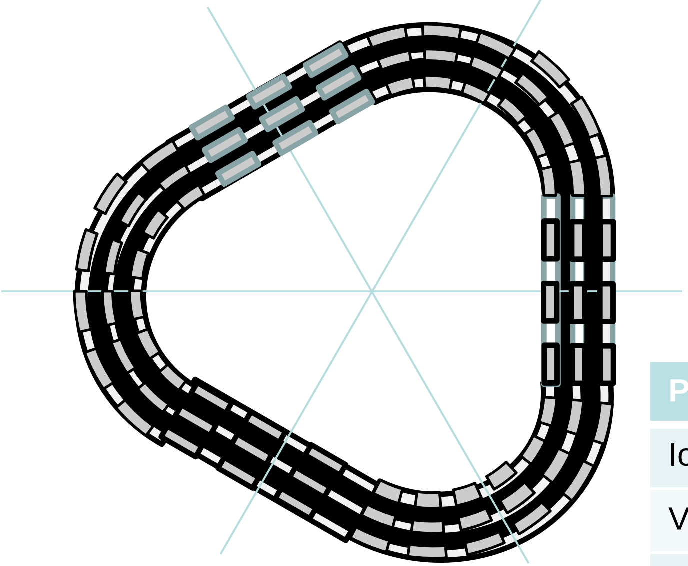
Kevin Brown BNL SRQC concept

Design of a Storage Ring QC



PALLAS Style Circular Ring

Parameter	Value	Units
Ion	$^{7}Li+$	
Velocity	1000	[m/s]
RF Freq.	12600000	[Hz]
Circum. (C)	1	[m]
$L = \beta\lambda = 2\pi v_0/\Omega$	0.07936508	[mm]
$\omega_{sec} \equiv \omega_\beta = 2\pi v_0/\lambda_\beta$	5909802.49	[Hz]
P=C/L	12600	
Q = C/λβ = ωsecC/2πv0	940.574279	
P/Q	13.3960712	
$D0 = R/Q^2$	1.799E-07	[m]
drive energy ratio (q)	0.21113856	



Triangular Ring

Parameter	Value	Units
Ion	$^{171}Yt^{+}$	
Velocity	200	[m/s]
RF Freq.	18,900,000	[Hz]
Circum. (C)	2	[m]
$L = \beta\lambda = 2\pi v_0/\Omega$	0.010582011	[mm]
$\omega_{sec} \equiv \omega_\beta = 2\pi v_0/\lambda_\beta$	3,689,058	[Hz]
P=C/L	189000	
Q = C/λβ = ωsecC/2πv0	5871.3185	
P/Q	32.190385	
$D0 = R/Q^2$	9.23377E-09	[m]
drive energy ratio (q)	0.087866	

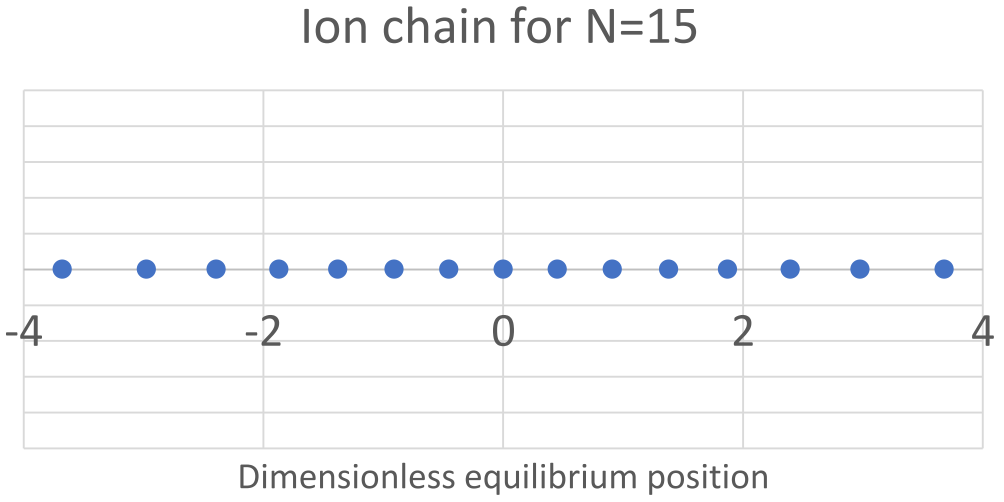
Kevin Brown BNL SRQC concept

A machine learned model for quick access to analytic solutions of a QIS system

- The potential energy of this system is:

$$V = \sum_{m=1}^{N} \frac{1}{2} M \nu^2 x_m(t)^2 + \sum_{m \neq n}^{N} \frac{Z^2 e^2}{8\pi\varepsilon_0} \frac{1}{|x_n(t) - x_m(t)|}$$

- Ions are bounded to 1D by means of the EM trap field strength.



- The **equilibrium positions** of the *N* ions in the chain can be determined from:

$$u_m - \sum_{n=1}^{m-1} \frac{1}{(u_m - u_n)^2} + \sum_{n=m+1}^{N} \frac{1}{(u_m - u_n)^2} = 0\,; \;\; m = 1, 2, \ldots, N.$$

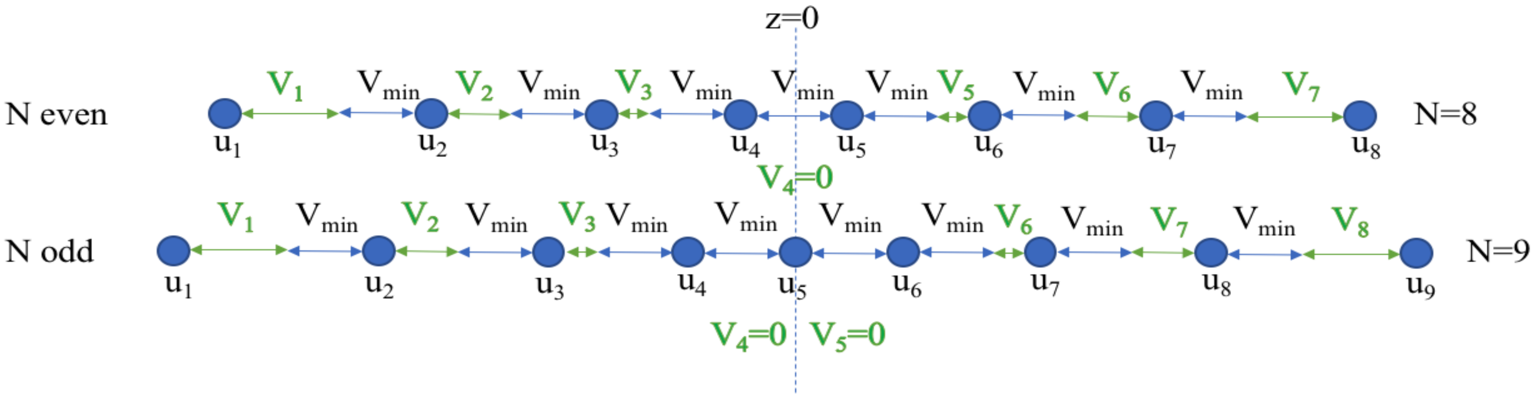
  – A function of the number of ions *N.*

  – Determined by solving a system of *N* coupled non-linear algebraic equations.

D.F.V. James, Appl. Phys. B 66, 181-190 (1998)

A machine learned model for quick access to analytic solutions of a QIS system

- We are interested on a chain with a large number of ions and in multiple dimensions.
- The numerical calculation quickly becomes impractical for large N.
- This problem can be formulated in terms of the minimum separation between ion.
  - This reduces the numbers of variables



Bohong Huang, Clio Gonzalez, Trudy Bolin, Aasma Aslam, Salvador Sosa, Sandra Biedron, Kevin Brown, “AI-assisted design and virtual diagnostic for the initial condition of a storage ring quantum information system,” manuscript in preparation for IEEE Access.

Towards a digital twin of the SRQC

- The control of individual ions needs to be very precise for QC applications.
  - Lasers need to operate on individual ions within the ICC.
  - **We don't necessarily have diagnostics available that provides individual ion positions.**
- We use a **ML model that predicts the positions of ions** in arbitrary sized ICCs.
  - Scaling of different analytical solutions so they can be compared against each other.
  - Fitting to a functional model.
  - The ML model predicts the fitting parameters.
- Ion positions can be reconstructed from this ML approach.
- This component needs to be integrated into the overall systems engineering design and will be used for control of the SRQC.

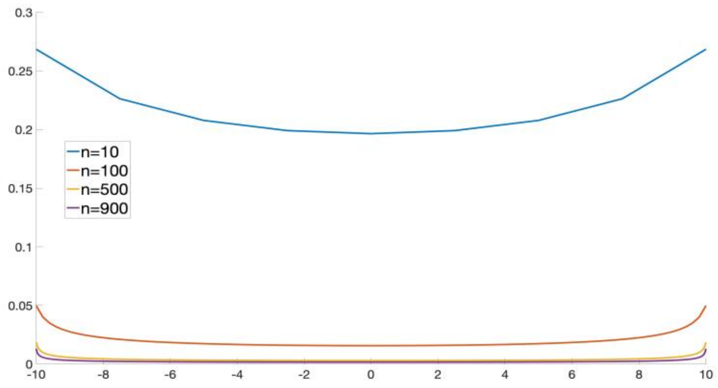


Fig. Analytical solution for different sized 1-D ion chains (N=10,100,500,900). Scaled position vs. ion spacing.

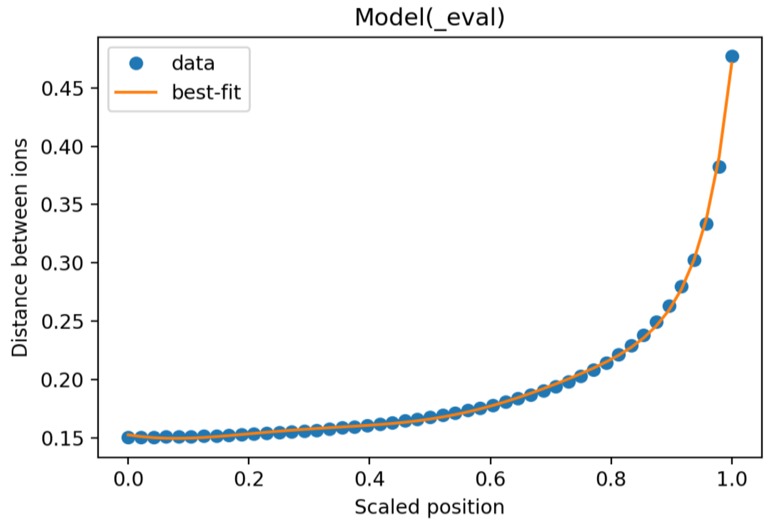


Fig. Analytical solution and model fit to one half of the N=200 ion chain.

Bohong Huang, Clio Gonzalez, Trudy Bolin, Aasma Aslam, Salvador Sosa, Sandra Biedron, Kevin Brown, "AI-assisted design and virtual diagnostic for the initial condition of a storage ring quantum information system," manuscript in preparation for IEEE Access.

Free-Electron Lasers

- Free Electron Lasers (FELs) at many wavelengths have enabled new developments in a broad range of disciplines.
- Highly successful as measured by their subscription rates.
- Driver of the FEL is an electron beam linear accelerator (linac).
- Need for higher electron beam energies capable of generating higher energy X-rays for activities such as high-energy density physics
  - linac becomes longer
  - costs quickly become prohibitive (state of art accelerating technology needed)
- One way of reducing the costs of such a longer linac is to
  - **reduce the size of the cavities**
  - **high-gradient of acceleration**
- Compact accelerating structures are also high-frequency, (C and X-bands)

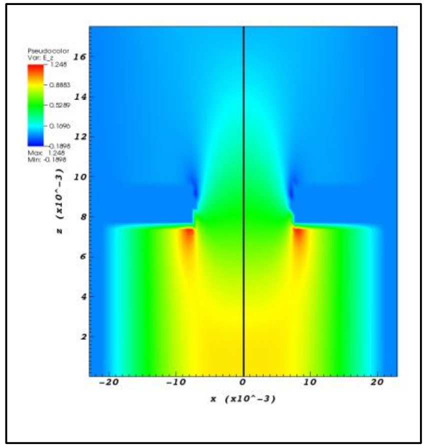
UCLA leading a compact FEL effort; ***we have a focus on MBSE of the entire system relying heavily on HPCs and AI/ML and DTs***

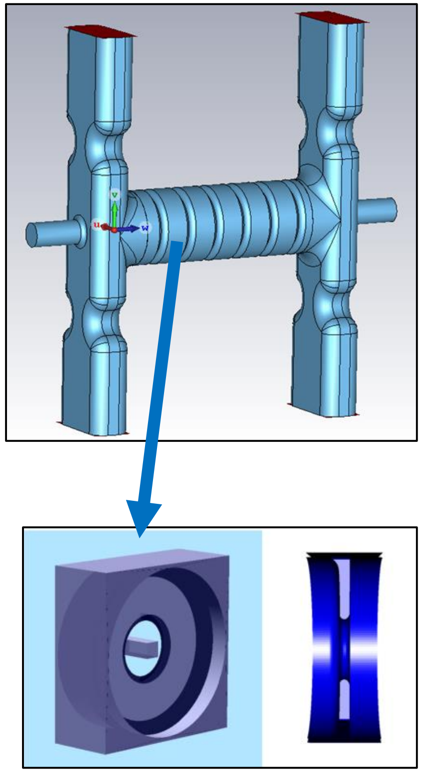
Need is growing as is the need for combinations of several dynamical system RIs

Example pieces C-band Cryo-cooled Accelerator Design

- Develop cavity/linac design using cryo-cooled technology for future FEL applications (such as UC-XEL and MaRIE)
- Achieve high gradient via cryo-cooling (reduce linac length for limited space)
- Cooling the cavities to cryogenic temperatures, (c.a. 77 K) reduces
  - surface resistance
  - thermal expansion coefficient
- Some things to consider
  - power requirements, cooling costs vs. current FEL designs, constant gradient, constant impedance, HOM dampers, peak fields, heating, breakdown rate, tolerances, frequency stability
  - …etc.

Parameter	Value	Units
Frequency	5.712	GHz
Cell length	17.495	mm
Outer radius	21.13	mm
Iris radius	7	mm
Phase advance	$2\pi/3$	rad





C-band structure electric field distribution

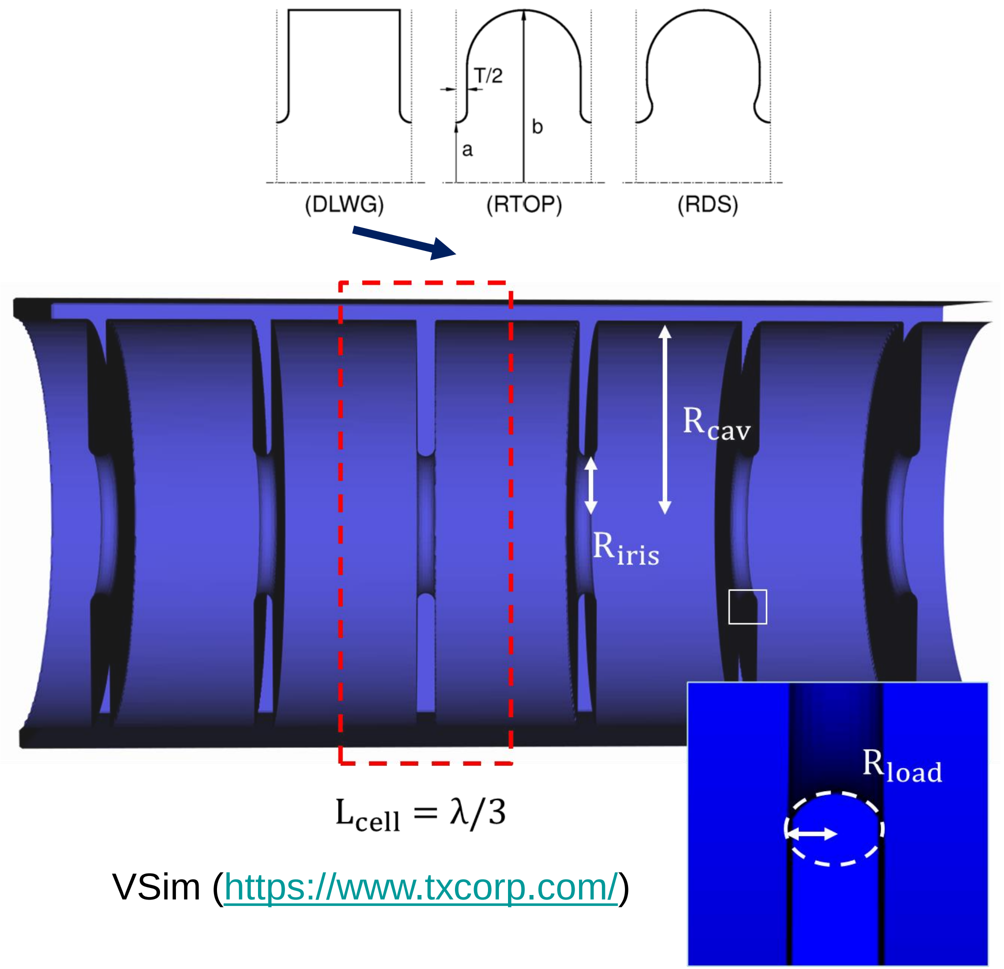
From 10th Int. Particle Accelerator Conf. IPAC2019, Melbourne, Australia
ISBN: 978-3-95450-208-0 doi:10.18429/JACoW-IPAC2019-MOPTS117

Next Steps

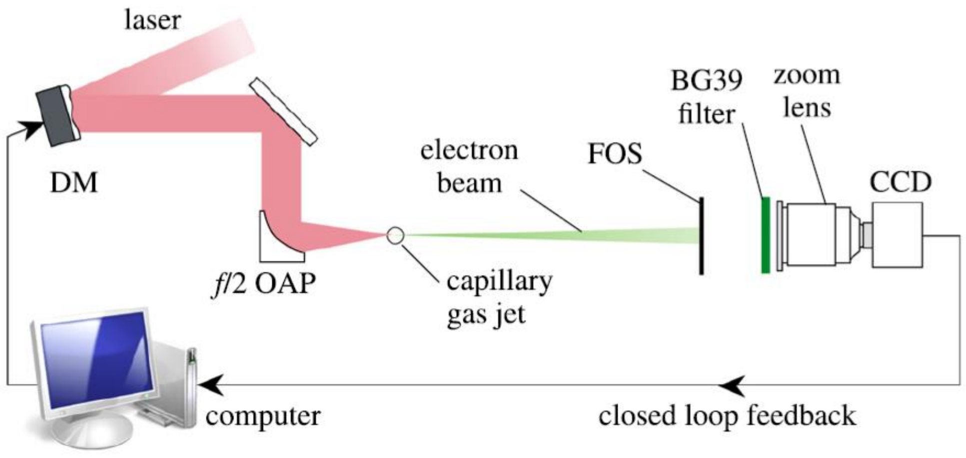
Fix model after RF structure down-select

- Present design assumes SLAC-type 3-m S-band structures
- MaRIE will use newer designs
  - — Improved shunt impedance
  - — Different lengths
- New wakefields will require lattice retune
- Overall momentum chirp reduction
- Sensitivity studies (esp. with t-cavities)
- High-charge studies
- Basic transport
- Multibunch / interleaving methods
- ***Model comparisons***
- ***Diagnostics support (test stand design)***
- e.g. working on upgrading **modeling software**
- Adding space in current lattice model
- Determining required performance
- Modeling proposed systems
- Cut copper
- Testing with RF and Beam
- Update this piece of the overall system's model/DT

Possible cell profiles



Convolutional neural network-based modeling of an ultrafast laser driving a LWFA

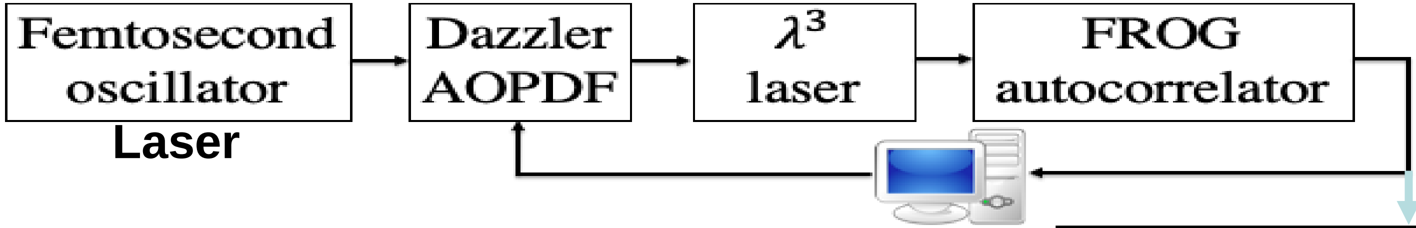


- This model was developed by means of feed-forward back-propagation neural network using second, third and fourth-order input phase, and hole position, width, and depth as input parameters.


Settings_Shot0.txt - Notepad
File Edit Format View Help
```
# order2, order3, order4, hole position, hole width, hole depth
-7.230165840892783509e+03
-2.448630147639668576e+04
2.773882107848635581e+05
7.647533868021170865e+02
7.808658269726640810e+01
3.895090516068982222e-01
```

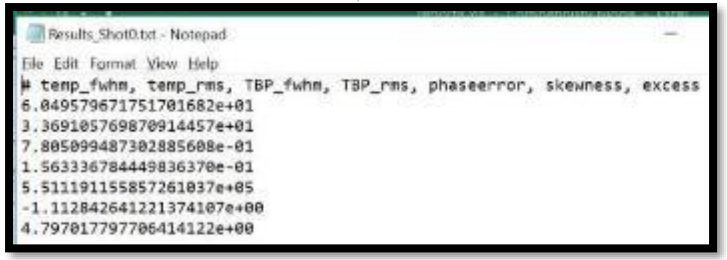
Femtosecond Oscillator: A setup for generating ultra-short laser pulses.

Dazzler AOPDF: The Dazzler system is an acousto-optic programmable dispersive filter. It enables the separate control of both the spectral amplitude & the spectral phase.



Will apply on Michigan system in Summer 2021 as a controller

- Lamda Cube Laser: Focuses the laser within a volume of cube of the laser wavelength, to concentrate intensity of the laser.
- Frog Auto-Correlator: Measures different parameters of the laser after passing from lamda cube, presented in reportR file, like fwhm, rms etc. Frequency resolved optical gating, used to temporary characterize the pulses. It enables both the phase and the amplitude of the pulse be retrieved simultaneously.

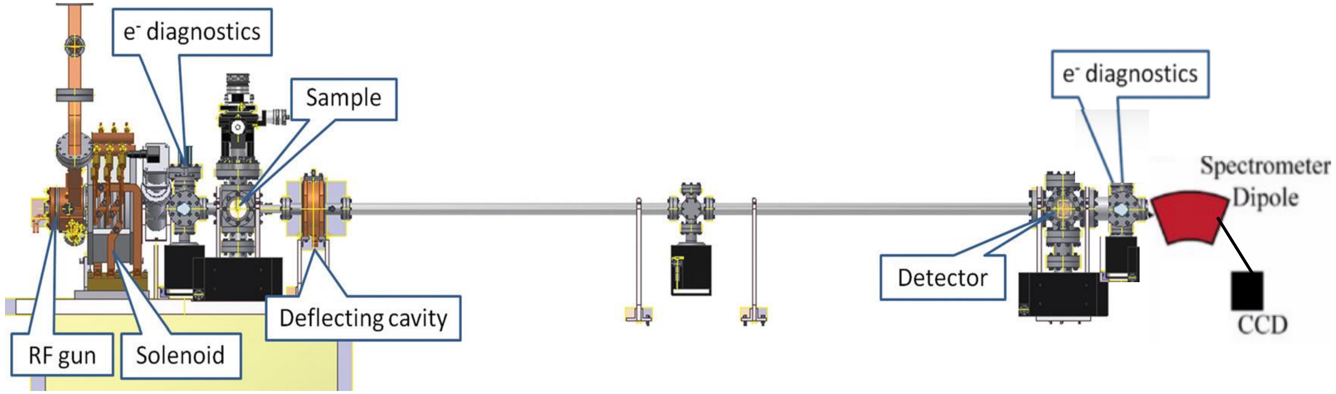

Results_Shot0.txt - Notepad
File Edit Format View Help
```
# temp_fwhm, temp_rms, TBP_fwhm, TBP_rms, phaseerror, skewness, excess
6.049579671751701682e+01
3.369105769870914457e+01
7.805099487302885608e-01
1.563336784449836370e-01
5.511191155857261037e+05
-1.112842641221374107e+00
4.797017797706414122e+00
```

Newest Programs

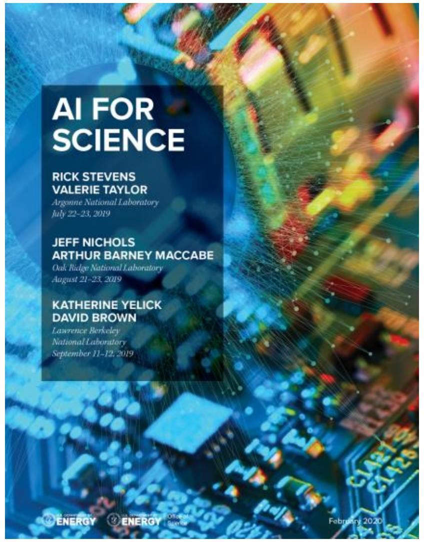
- Materials Discovery
- Beam Target Health

Materials - Two DOE facilities are involved: ATF MUED and ALCF

Accelerator Test Facility (ATF)



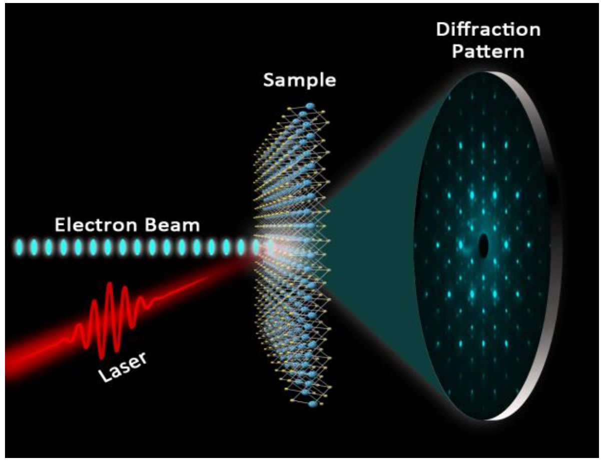
Argonne Leadership Computing Facility (ALCF)



The combination of machine hardware, advanced computing for simulation, and data science for surrogate modelling, training of neural networks and data analysis is inspired by our past work and our participation on DOE meetings, workshops and reports such as AI for Science (*https://www.anl.gov/ai-for-science-report*).

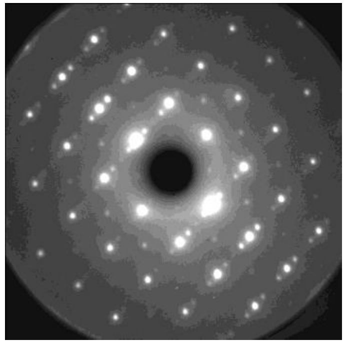
What is MeV ultrafast electron diffraction (MUED)?

It is a pump-probe structural measurement technique for exploring time-resolved, ultrafast processes in different material systems.

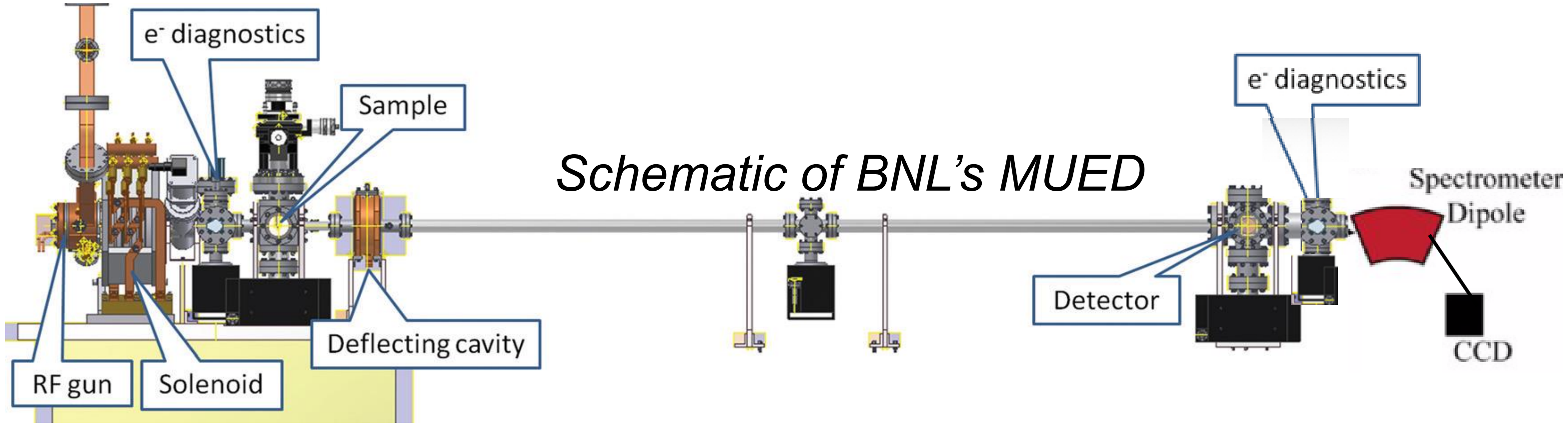


Courtesy Jing Tao, BNL

- ✓ High scattering cross-section
- ✓ Extremely short wavelength (diffraction patterns contain many reflections)
- ✓ Reduced space charge effects
- ✓ Less multiple scattering effects



Courtesy Jing Tao, BNL



Schematic of BNL's MUED

Source parameters for typical operation

Beam energy	3 MeV
N e- per pulse	1.25×10^6
Temporal resolution	180 fs
Beam size diameter	300 (100 best) µm
Max repetition rate	5 – 48 Hz
N e- per sec per µm^2	88-880

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Automatic characterization of materials from MeV Ultrafast Electron Diffraction patterns

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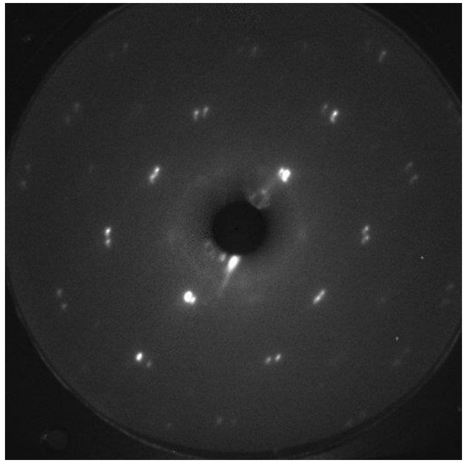
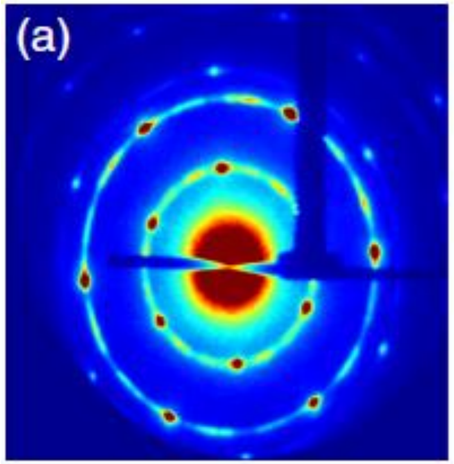
Examples:

- Black phosphorus thin films



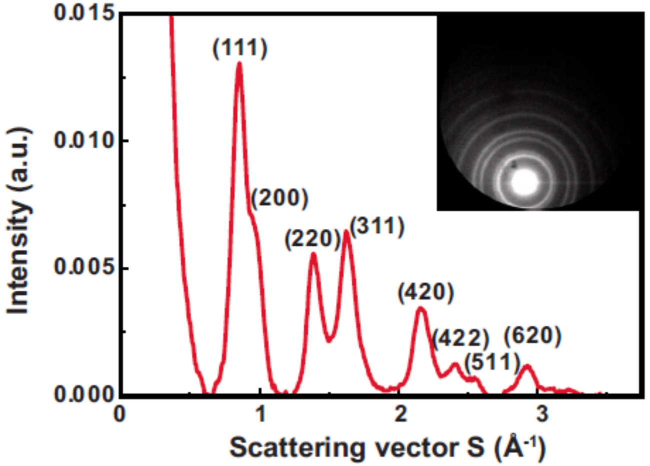
Courtesy of Junjie Li and Jing Tao, measured at BNL

- Graphite thin films



Harb, M., et al. PRB 93.10 (2016): 104104.

- Polycrystalline gold films



Ligges, M., et al. APL 94.10 (2009): 101910.

✓ Material samples are available to use at BNL

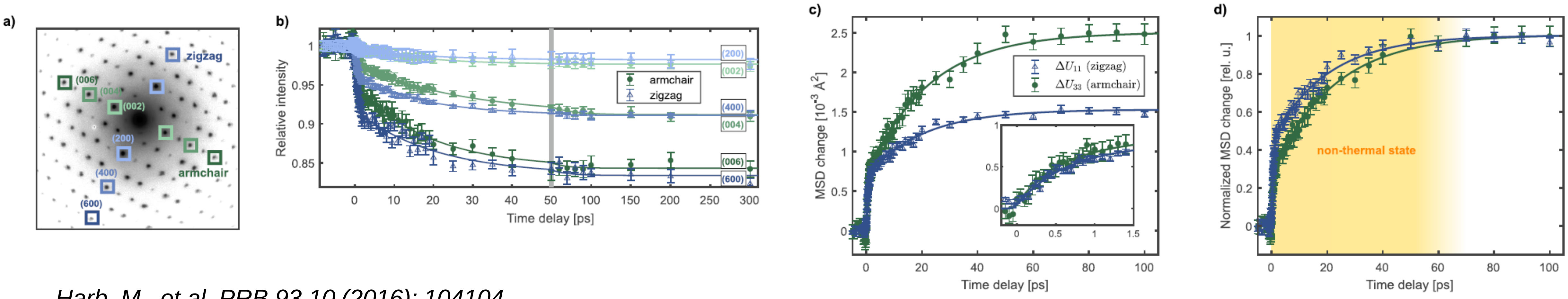
✓ All these materials have previously been measured by MUED and good quality diffraction patterns were obtained.

Automatic characterization of materials in synergy with laser and beamline control

- We will also fully characterize these materials systems employing different laser fluences, pulse delays and sample temperature.

- Faster alignment and improved control of electron beam achieved before will provide better quality measurements, allowing further research on these material systems.

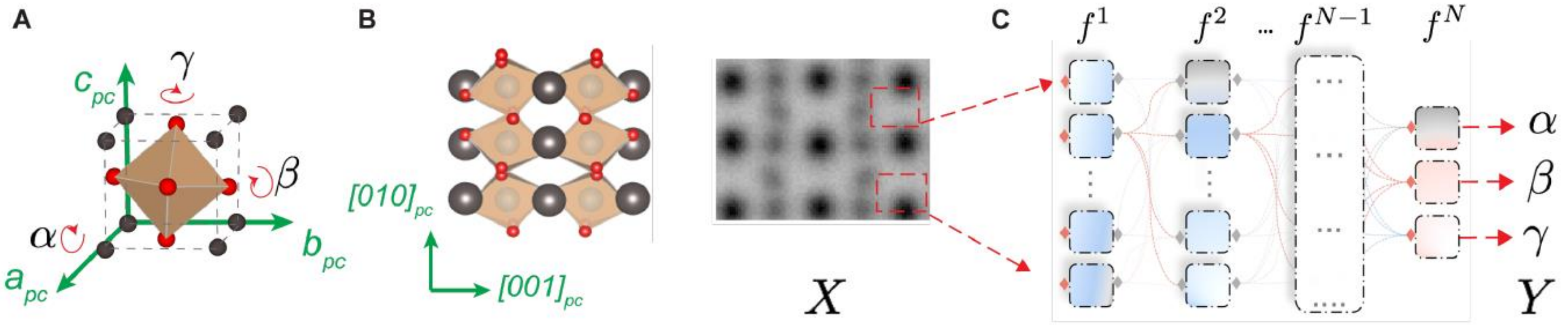
- *Example:* lattice dynamics black phosphorus previously analyzed with 70 keV UED



Harb, M., et al. PRB 93.10 (2016): 104104.

Analysis automation and database creation

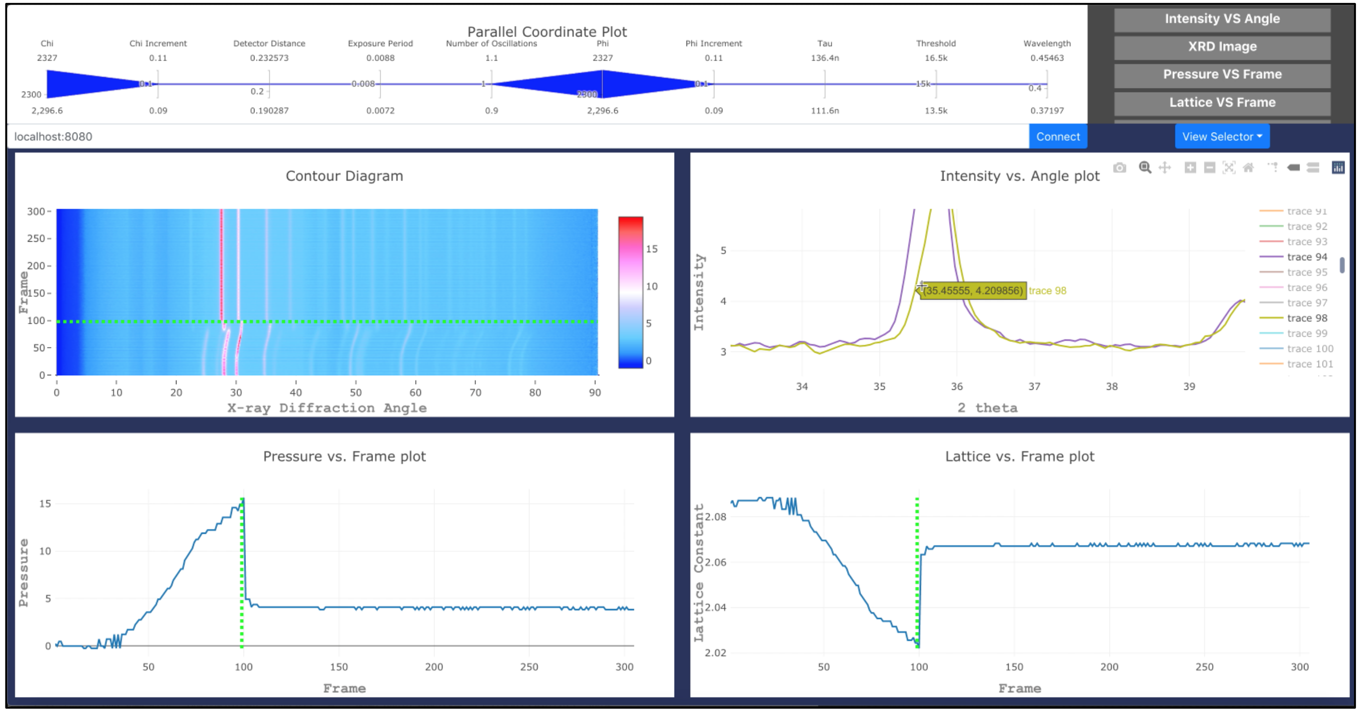
- *These proposed goals involve offline experiments (no instrument time).*
- Analysis of collected diffraction patterns with software available at BNL.
- Automation of this process can lead to real-time analysis. Similar control methodologies on lasers on the main ATF and the MUED by other members of our team.
- We will also implement artificial neural networked based models to extract relevant information and predict the materials structure.
- Relevant previous work on STEM by Nouamane Laanait (ex ORNL) et. al.:



Laanait, Nouamane, Qian He, and Albina Y. Borisevich. arXiv preprint arXiv:1902.06876 (2019).

Analysis automation and database creation

- We will incorporate the use of data visualization tools such as *Cinema:Bandit* (by Sweeney et. al. at LANL)



- Another similar framework developed at ORNL: *Universal Spectroscopic and Imaging Data (USID)*
  - Represents data in a standardized manner.
  - HDF5 data format to facilitate storage of large data.
  - Free open-source Python packages to access and analyze datasets.

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Non-destructive real-time diagnostic

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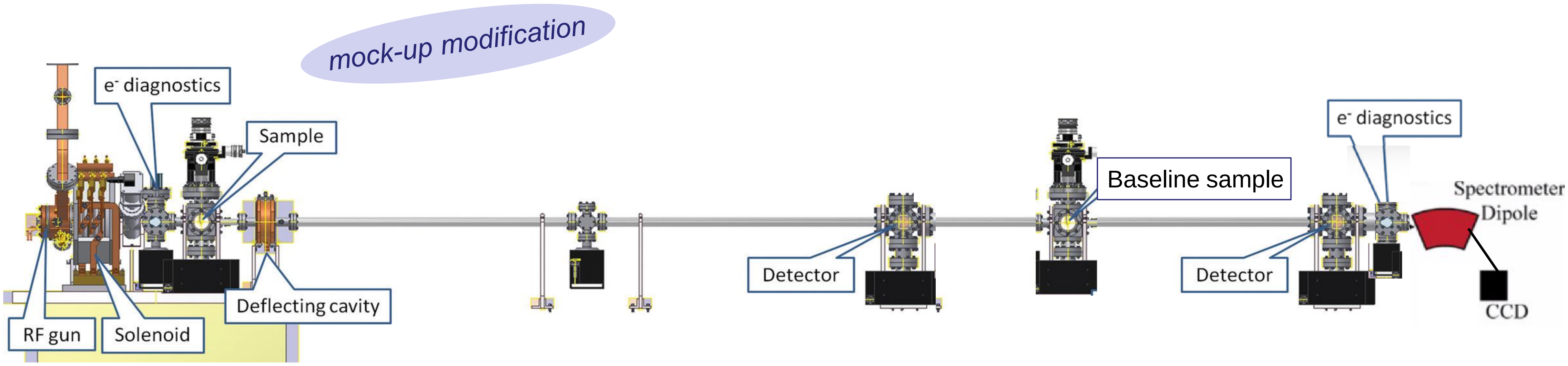


- Collected diffraction patterns can be fed into our virtual diagnostic developed previously to infer beam parameters.
- Shot-to-shot control of the beam can be implemented using this diagnostic.

Goal: ensure beam stability during single shot measurements with minimum down time of the machine and minimum intervention of the operator

Non-destructive real-time diagnostic

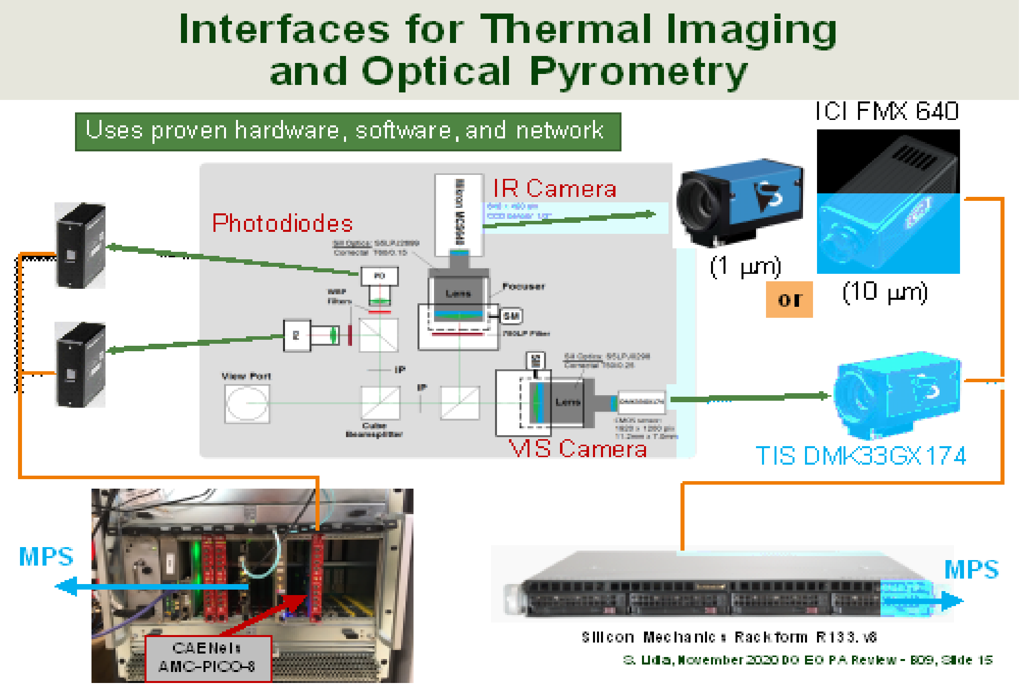
Ultimate goal: achieve single-shot capabilities for MUED

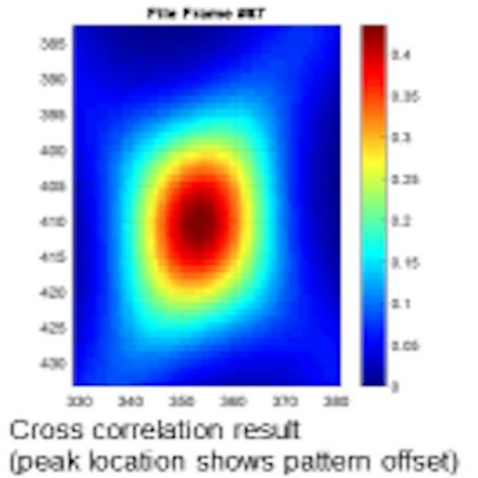
- Single-shot MUED will enable higher instrument throughput, measurement of samples that are susceptible to pump or probe damage, and potentially higher precision
- Integration of many shots to obtain good S/N ratio limits precision (high-frequency noise sources and systematic errors)
- The full suite of diagnostics described would enable complete pump-probe characterization (pump-probe delay, pump energy, probe charge, probe energy, probe position)
- Normalization of single diffraction patterns to remove these noise sources then becomes possible, improving the precision of each single image, with or without subsequent averaging

Health of the target and beam dump at FRIB

- Using an edge-computing platform, we will interface with both the FRIB high-power target and beam dump's thermal imaging systems (TISes)
- Collecting the necessary data from the TISes for a variety of beam conditions as well as monitoring the health of the target and beam dump.
- Using this information to create a model to predict health and identify operational issues through local (edge) and HPC computing resources.
- The model can be updated through this edge network as well as other computing resources and stored locally.
- This is intended to be a dedicated system interfaced to EPICS through the framework being created by our team.

Starting now!





The FRIB TIS imaging systems (left) and the illumination of the vibrational modes in the beam target using cross-correlation analysis (right)

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AI Institute for Enhancing a Dynamic World

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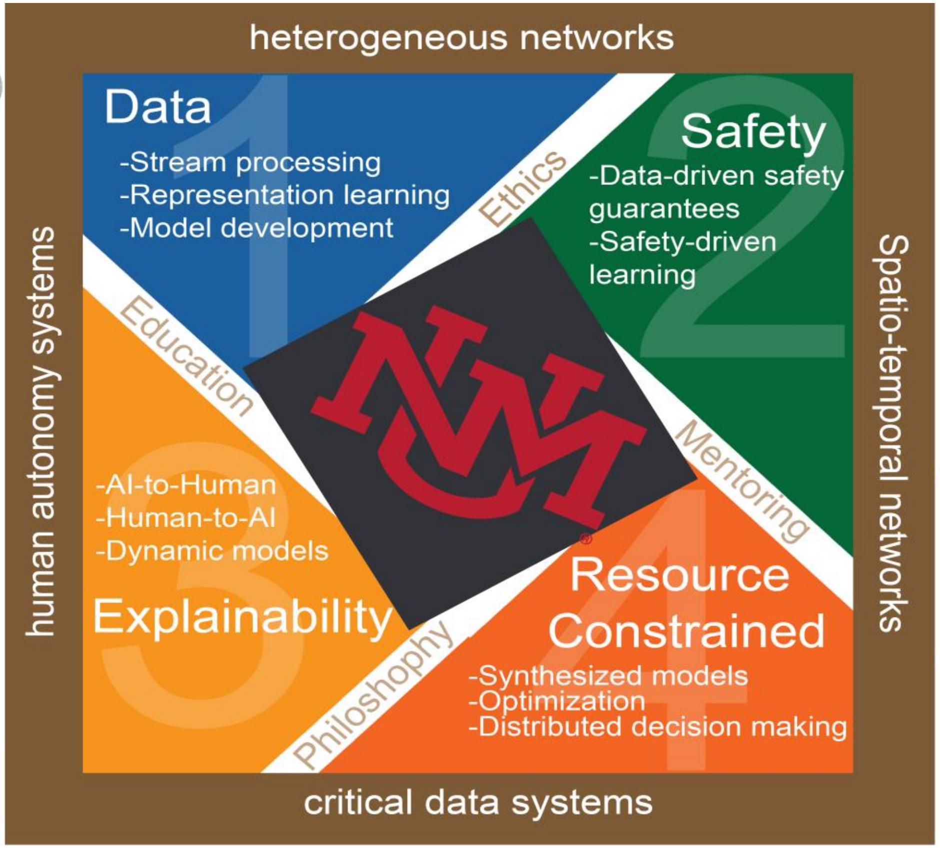

Lydia Tapia, CS

Sandra Biedron, ECE

Manel Martinez-Ramon, ECE

Abdullah Mueen, CS

Conclusions

- Many activities on-going in RIs involve systems that will be built and we are trying to provide prototype models (DTs) for the DT instances.
- In RIs, not many DT Aggregates except transferring some information between related systems.
- **Looking forward to more discussions through the rest of the workshop and thoughts and collaborations for our deployed or to be deployed projects that rely heavily on models with of hopes of achieving an even better model.**
- ***Some thoughts on edge computing lies in the appendices that I could not cover today with some examples.***
- We are happy to exchange and share many details – just get in touch! sgbiedron@elementaero.com

Thank you for your attention

We appreciate all the support from our additional inspiring team members, including

We also want to acknowledge our colleagues Dr. Christian Lavoie (*IBM Research*), Dr. Nouamane Laanait, Dr. Alan Tennant (*Oak Ridge National Laboratory*), Dr. Marek Osinski (*Center for High Technology Materials, UNM*), Dr. Timothy J. Bunning (*Air Force Research Laboratory*), Dr. Kevin Jensen (*Naval Research Laboratory*), Dr. Jeffrey Nelson (*Center for Integrated Nanotechnologies, Sandia and Los Alamos National Laboratory*), Dr. Malachi Schram (*Pacific Northwest National Laboratory*), Dr. Aric Hagberg (*Los Alamos National Laboratory*), Dr. Frank Alexander (*Brookhaven National Laboratory*), David Womble (*Oak Ridge National Laboratory*), Hassan Hafizi (*Los Alamos National Laboratory),* and Andreas Waechter *(Northwestern)*

Things we need for the edge - *Methodologies*

- Problems
  - Large quantity of data, difficulties for storage over time.
  - Data non-labelled or categorized

- Questions
  - How much data is needed to capture its probabilistic properties needed to train?
  - The data at different time instants, is wide sense stationary (WSS), or time varying?
  - Can I extract information from non-labelled data?

Things we need for the edge - *Data discrimination*

- Should I store or discard this data?
  - Assuming WSS data, models exist (Gaussian mixture models, Markov Random fields, others) to keep or discard the data depending on its likelihood.
  - If cyclostationarity is assumed, then bayesian methods exist to select the data from a database to train a structure depending of their similarity with the test sample.

Things we need for the edge - *Why online training*

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- WSS data
  - Samples can be used for training once and then discarded: future samples will contain the same information.
- Non stationary data:
  - Samples must be used once and then discarded. The learning process must contain a forgetting factor.
  - In some cases, the structure must be adaptive itself: the system must be able to drop parts of its structure when they are not needed (sparsity).

Things we need for the edge - *Adaptive strategies*

- They are classic and well known. Some linear supervised examples are:
  - Least mean Squares (Widrow and Hopf, 1960)
  - Recursive Least Squares (Plackett, 1950)
  - Kalman filters
- Modern nonsupervised adaptive techinques include
  - Clustering
  - Restricted Boltzmann Machines, autoencoders (Hinton & Salakhutdinov, 2006)
- They are based on gradient descent approaches.

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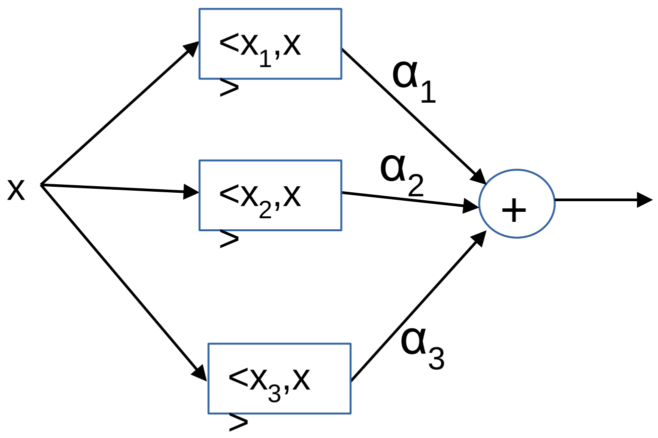
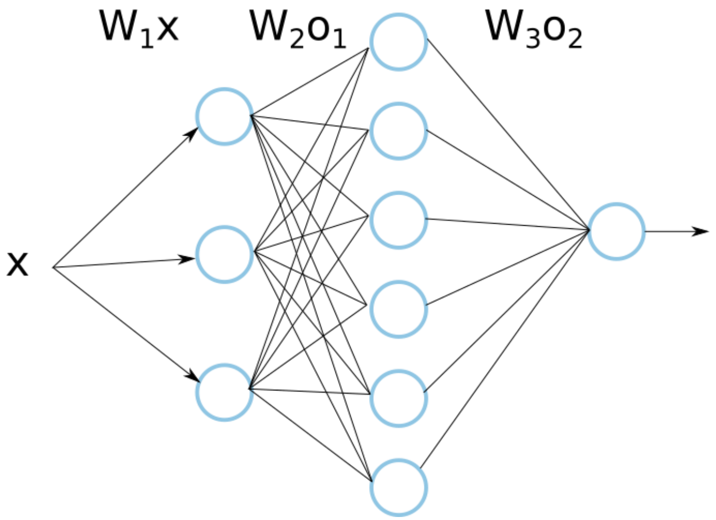
Things we need for the edge - *Online trainability of structures*

- Two types of structures: shallow and deep.



Dual representation of a shallow structure. All linear estimators admit this representation. Most nonlinear ones *only* admt this one. Grows with training data.



Deep structure. It only admits a primal representation. Dimensions of matrices W_i are fixed. It does not grow with the training data.

- Shallow learning
  - Efficient, explicit control of generalization (Vapnik and Chervonenkis, 1997). Good of rlow data.
  - Dual representation (Schoelkpf, 2001) allows straightforward nonlinear versions. Existence and uniqueness of solutions (Mercer’s Theorem, Aizerman et al, 1964)
  - Expressed as a function of NxN matrices, that grow with the number of data: bad for large data.
  - They only admit block training (not online)
- Deep structures
  - Higher structural complexity, not explicitly controlled.
  - Always expressed in primal spaces: matrices do not grow with the data.
  - They can be trained in block or online.
  - The adaptation speed depends on the complexity.

Things we need for the edge - *Online training concept*

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- It has its roots in gradient descent.
- The learning criterion includes the minimization of an error (e.g MMSE) or an information measure (cross entropy).
- The parameter adaptation rule can be expressed as

$$\Delta w_{ij}^{n} = \frac{\delta e}{\delta w_{ij}^{n-1}} \qquad\qquad w_{ij}^{n+1} = w_{ij}^{n} + \mu \Delta w_{ij}^{n}$$

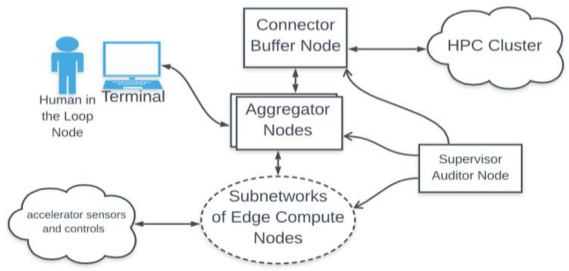
  - Where e is the error or info measure. It can be implemented using the well known back propagation algorithm.
  - e can be computed from the average of one training data or batch, thus the online training is natural in gradient descent.
  - The rule can include a forgetting factor.

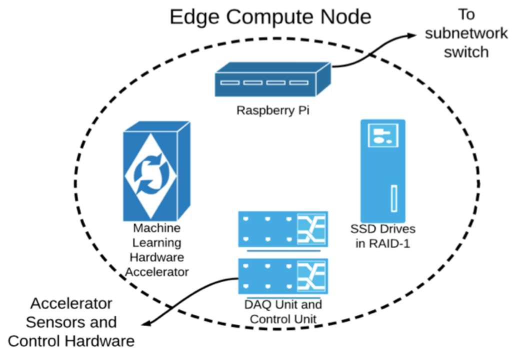
Things we need for the edge - *Training speedup*

- A deep structure is typically slow and it requires many training iterations.
- The training time increases with the structural complexity.
- In order to speedup the process, several techniques have been proposed in the literature:
  - Online selective training of the data.
  - Adaptive selection of the neural network structure.
  - Data augmentation.

Things we need for the edge - *INCLUDING for Large, complex systems*

- HPC and control center might be far away.
  - Need local computing, new computing hardware, new computing architectures, and co-proccessors for fast inference.
  - Local models to be updated or portion of the entire system model need to be updated.
  - Need to pass data back to HPC and main control (what frequency etc TBD)
  - Local storage.
  - Real time, on or near sensor ASICs, FPGAs
  - Ability to control locally

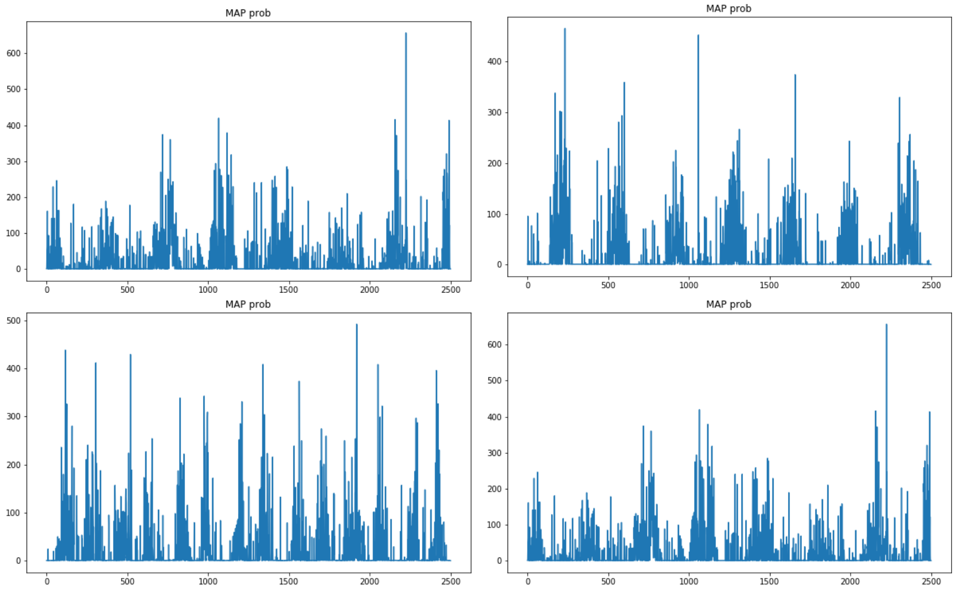




"Athena" Controls Suite [ATHENA - Accelerator Technologies, Human, Edge-computing, and Neural-network Attribute - Controls Suite, Element Aero, manuscript in preparation]

- Data selection in cyclostationary environments, e.g. electrical loads
- Example of a life saving system with humans in the loop; fire segmentation in thermal imaging for situational awareness. Neural network procedures can fully characterize the fire ground by producing natural language descriptions of the scene. The method must be real-time and unsupervised
- An autonomous satellite
- Big scientific systems and sub-subsystems
- Data from high-energy physics experiments
- and a concept system for a museum for environmental control/exhibit/security.

Data selection in cyclostationary environments



Training data similarities over 7 years for four different test samples chosen at random from fall, spring, summer and winter seasons.

Pereira, Martínez-Ramón et al, IEEE Transactions in Smart Grid

- Bayesian methods are used to characterize electric load data.
- A probabilistic similarity is used to select training data similar to the present test data.
- Low complexity machines can be trained with selected data ad-hoc for every test data.
- Tested in 24 hours ahead electric load forecast with data from Maine, New Hampshire,Vermont, Connecticut, Rhode Island, Massachussets. Improves performance in all tested predictor structures.

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Online unsupervised learning in fire characterization

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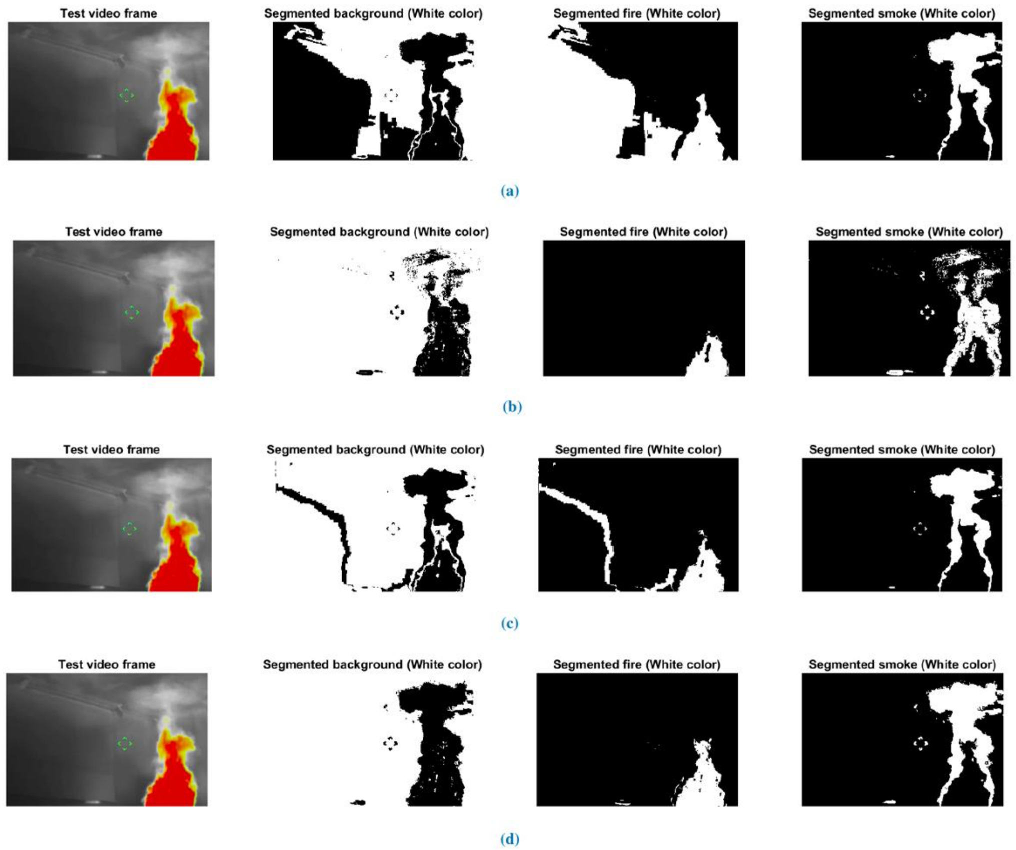

- Online training for fire, smoke and background detection in IR sequences
- Features are intensity, velocity, divergence and vorticity for every pixel.
- Random Markov fields (d) provides best performance

Ajith and Martínez-Ramón, IEEE Access, vol. 7, 2019.