Closing of the workshop

“1st MODE Workshop on Differentiable Programming for Experimental Design”

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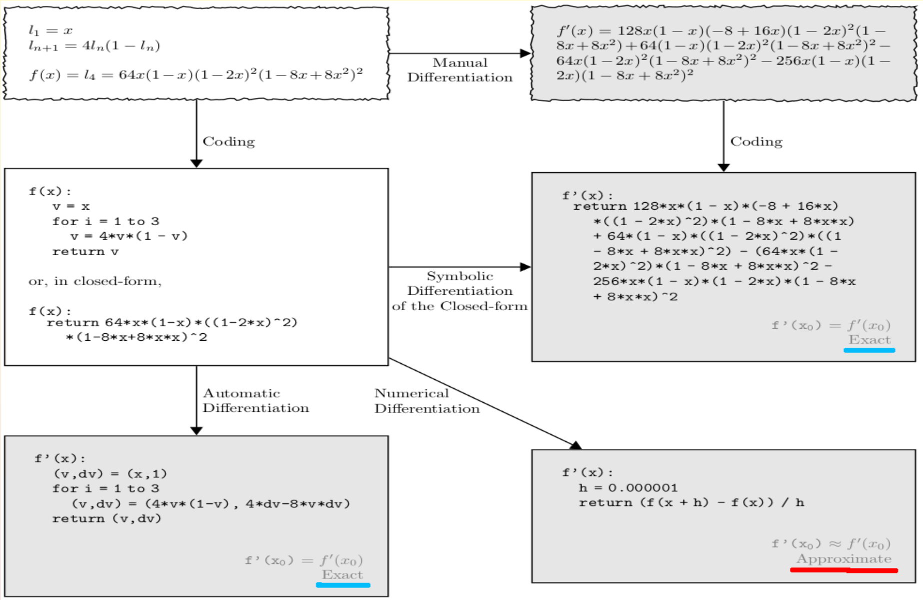
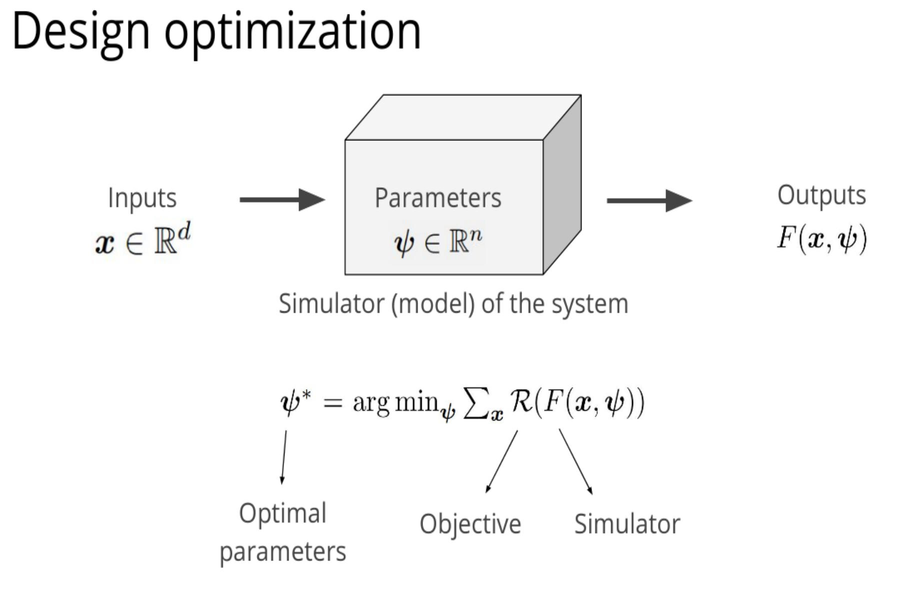
First MODE Workshop

- Opening Lecture: Differentiable Programming and Design Optimization (Atilim Gunes Baydin, U. Oxford)



Automatic differentiation

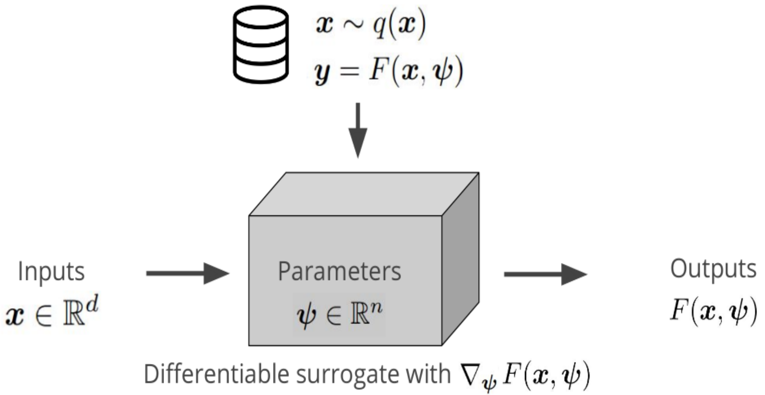
- Opening Lecture: Differentiable Programming and Design Optimization (Atilim Gunes Baydin, U. Oxford)



- Opening Lecture: Differentiable Programming and Design Optimization (Atilim Gunes Baydin, U. Oxford)

Surrogates for differentiability

- Use the dataset to learn a differentiable approximation of the simulator (e.g., a deep generative model)



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Optimization of experimental design

- Design of instruments is a complex task, involving a combination of performance and cost considerations
- We need the next generation of tools to optimize modern and future particle detectors and experiments
- MODE (Machine-learning Optimized Design of Experiments) collaboration!

  https://mode-collaboration.github.io/

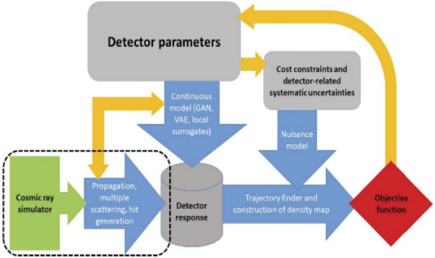
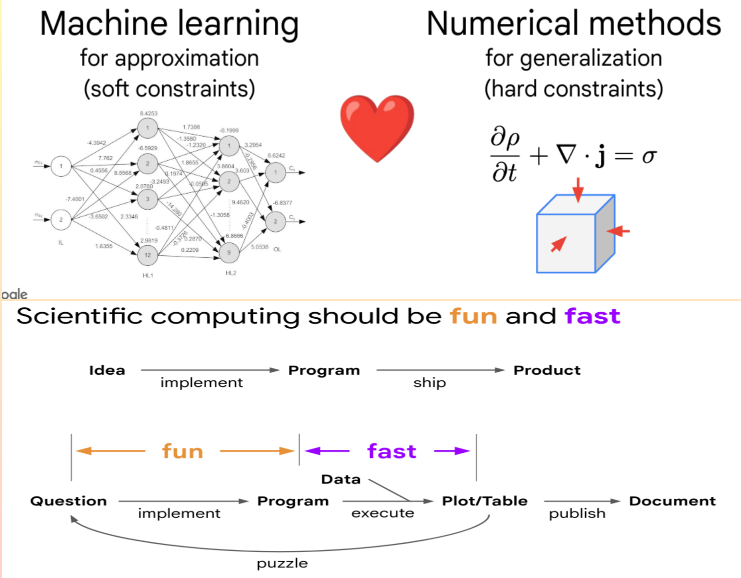


Figure 1. *Conceptual layout of an optimization pipeline for a muon radiography apparatus. Modules within the dashed black box inform the validation of a continuous model and are not part of the optimization flow.*

Baydin, Cranmer, de Castro Manzano, Delaere, Derkach, Donini, Dorigo, Giammanco, Kieseler, Layer, Louppe, Ratnikov, Strong, Tosi, Ustyuzhanin, Vischia, Yarar. 2021. "Toward Machine Learning Optimization of Experimental Design." Nuclear Physics News 31 (1)

- Keynote Lecture: JAX for Scientific Computing (Adam Paszke, Google Research, Brain Team)




```
jit(vmap(grad(odeint(jet(model)))))
```

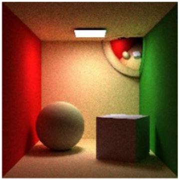
- Keynote Lecture: JAX for Scientific Computing (Adam Paszke, Google Research, Brain Team)

Should you consider Dex?

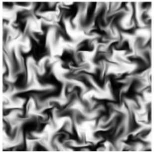
1. Your problem is difficult to express in array DSLs
2. You are comfortable working with research software (but with support)

📞 Let us know if it sounds interesting! We're looking for a small group of pilot users.

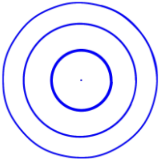
Ray tracing



Fluid simulations



n-body simulations



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- Keynote Lecture: JAX for Scientific Computing (Adam Paszke, Google Research, Brain Team)

JAX	Dex
NumPy	Explicit loops
Acceleration	Acceleration
Differentiation	Differentiation
Batching	Batching
Scaling	🚧 Scaling
Scientific computing helpers	🆘 Scientific computing helpers 🆘
💪 Battle tested	🧑‍🔬 Research software

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- Keynote Lecture: Generalization Properties of Deep Neural Networks Through The Prism of Interpolation (Mikhail Belkin, Halicioglu Data Science Institute, UCSD))

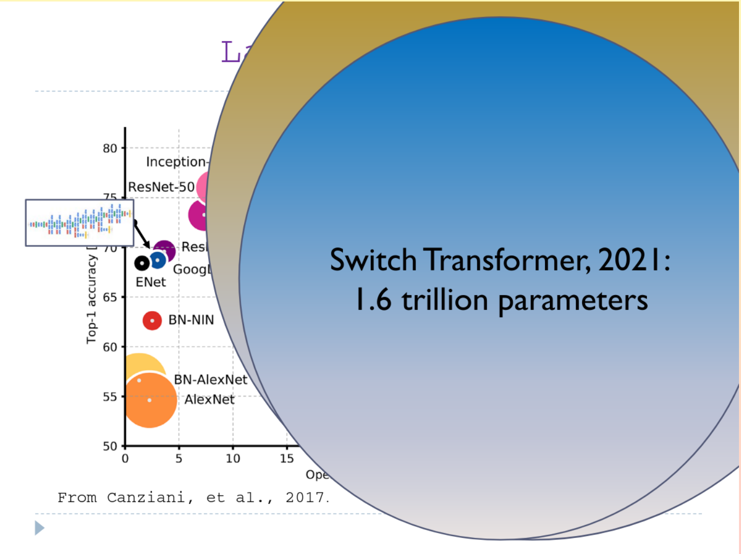
1. Generalization.

Why do neural networks generalize to unseen data?

2. Optimization.

Why can non-convex objective functions be optimized?

- Keynote Lecture: Generalization Properties of Deep Neural Networks Through The Prism of Interpolation (Mikhail Belkin, Halicioglu Data Science Institute, UCSD))



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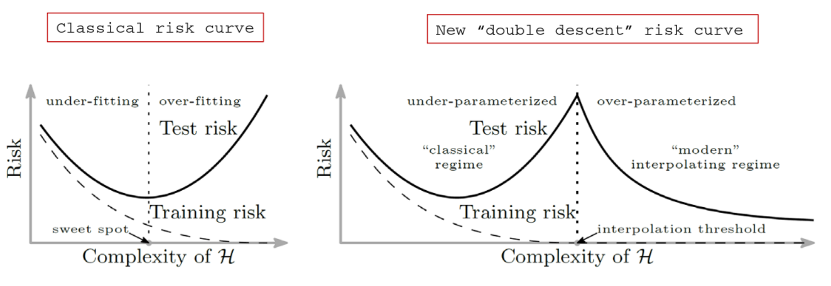

Overparameterized Systems

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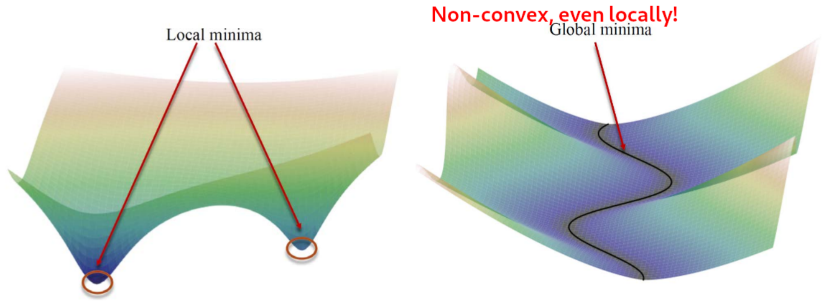

Classical underparameterized landscape $m \leq n$:

Isolated local minima

Overparameterized landscape $m > n$:

Manifolds of global minima

What is MODE about

- MODE is mostly about these people being right

$$argmax_{x,y}(\mathcal{L}(x,y)) \neq \left[argmax_x(\int \mathcal{L}(x,y)dy), argmax_y(\int \mathcal{L}(x,y)dx)\right]$$

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- *“We aim to create a versatile, scalable, customizable infrastructure, where a generic detector design task can be encoded, along with all the players (pattern reco, nuisances, cost constraints, a well constructed objective function).Then automatic scanning of the space of design solutions becomes possible!”*
- This doesn’t replace the work of the physicist! We aim at **extending the physicist’s abilities** by producing **design assistance tools**, focussing on **diagnostic tools and visualizations** for interpretability
- We don’t propose *the one optimal solution* to a given problem, we aim at proposing **a distribution of solutions** in a region of optimality, to assist design choices!
- Optimization targets are not only strictly physics-related (e.g. significances): we consider also **financial cost** and other constraints in the optimization

Begin simple, proceed towards complexity

- We identified and started studying some **relatively simple use cases**: muon tomography detector optimization, calorimeter optimization
- Plan to proceed to other simple use cases (e.g. small detectors for HL-LHC), providing **proofs of concept of increasing complexity**
- *"Every problem is difficult if you want to solve it well and make an impact"*
- In this workshop we aimed at starting to build **a community of interested peers** and identify **problems that we may tackle alltogether**

Want to join us? The door is open!

You are here today (in person or by avatar) because you worked at topics related to our research plan, or because you have an interest in doing so in the future.

So you look as close to the right audience as I can think of, when I say we need your help to improve the effectiveness of MODE.

I hope you will consider joining MODE, sharing research time and resources with us (e.g. help with coding, if you're still capable of that, or direct your students to our research topics, if you're a low-bandwidth senior!)

According to our Statute, becoming a collaboration member requires you to

→be interested in our research plan, and to produce research in that area

→bring competence of relevance, or vow to acquire it

→aim to contribute to it within your possibilities

Just send to the MODE steering board (Dorigo, Donini, Giammanco, Vischia, Ratnikov) a confirmation of the above and a short bio (or CV, or pointer to google scholar) and chances are we'll get you in!

Ideal flowchart:

1) One of the talks has identified an experimental need (for upgrade or initial design) which is impervious to common approaches, or for which it is clear that an end-to-end optimization could be **advantageous, feasible, and timely**
2) We consider possible ideas to attack the problem
3) We verify the absence of potential show-stoppers hard to overcome, as well as of efforts already ongoing at an advanced stage
4) We observe that some of us are potentially interested to develop original work in that area
5) This can lead to small groups of potential contributors, who are then free to organize their future activities

   - we then exert moral suasion to contributors to bring this within MODE, by becoming members of our collaboration

Of course, all of us are overbooked, so I don’t expect we can create ex novo several new groups

- **Opt-in** system, to be seen as a great opportunity: the effort is small (the length of the paper is constrained)
- White paper as **summaries of ideas** and a tentative road forward

Present status of the document

Divided in 6 sections

Content list of section 4 is still tentative - we will populate it with applications we care to describe, and on which we foresee future activities

Contents

Toward the End-to-End Optimization of Particle Physics Instruments with Differentiable Programming: a White Paper

MODE Collaboration
...

September 8, 2021

Abstract

Ideally each section should be at most 5 pages long. We want to target an agile 20–25 pages document.

The full optimization of the design and operation of instruments whose functioning relies on the interaction of radiation with matter is a super-human task, given the large dimensionality of the space of possible choices for geometry, detection technology, materials, and data-acquisition and information-extraction techniques, and the interdependence of the related parameters. On the other hand, enormous potential gains in performance over standard, "experience-driven" layouts are in principle at reach if an objective function fully aligned with the final goals of the instrument is maximized by a systematic search of the configuration space. The stochastic nature of the involved quantum processes make the modeling of these systems an intractable problem from a classical statistics point of view, yet the construction of a fully differentiable pipeline and the use of deep learning techniques may allow the simultaneous optimization of all design parameters.

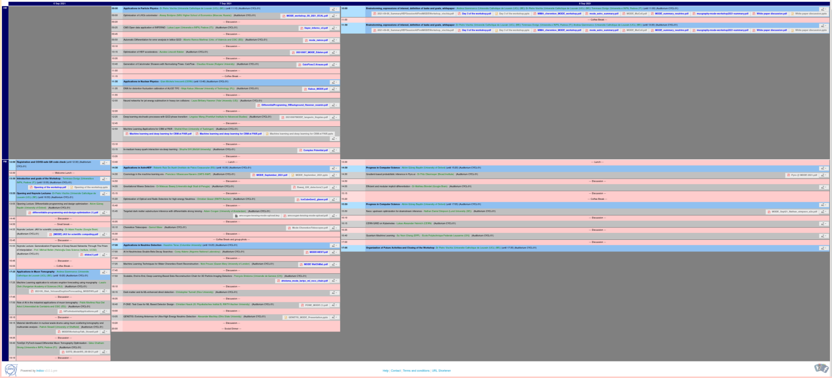
In this document we lay down our plans for the design of a modular and versatile modeling tool for the end-to-end optimization of complex instruments for particle physics experiments as well as industrial and medical applications that share the detection of radiation as their basic ingredient, and consider a selected set of use cases to highlight the specific needs of different applications.

Regardless of whether you'll be joining or not

- We'd be delighted (and **will definitely ping you by email**) if you would join an **open discussion session** of the next MODE Collaboration meeting!!!
  - Discussing ideas, opportunities, future work, and synergies, towards eventual collaborations!

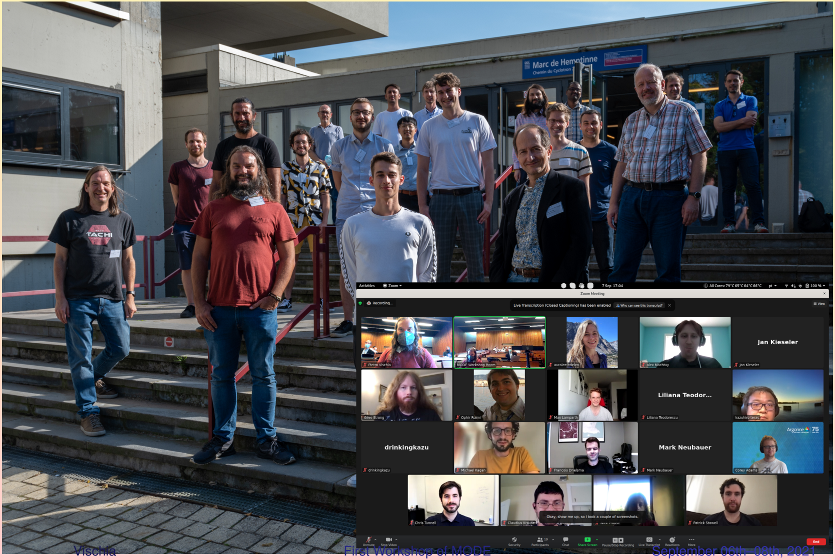
A final note on this workshop — 1

- It's great to be back, at least partially, to **in person discussions and brainstorming**
- Thank you very much to the Scientific Advisory Committee, the Organizing Committee (in particular to Carinne and Carine), and to all session chairs!
- Thank you very much to CP3 and UClouvain for permitting the workshop in this uncertain era, in particular to Christophe Delaere for the support as CP3 director!
- Thank you very much to the opening and keynote lecturers!
- Thank you very much to all the speakers of all the sessions!



A final note on this workshop — 2

- **Thank you, the participants, for the interest and the fruitful discussions**
  - A special thanks to the in-person participants for the courage of pioneering the return to in-person workshops
- **Now let's go and pioneer experimental design via automatic-differentiation-based optimization!!!...**



...and also let's maybe go for dinner!

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- We plan to go for sushi dinner at about 19:30: feel free to join!