Differentiable Simulation of a Liquid Argon TPC for High-Dimensional Calibration

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arXiv:2307.XXXXX

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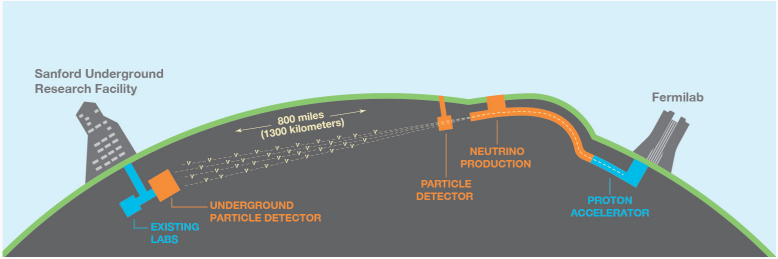
APC - CNRS

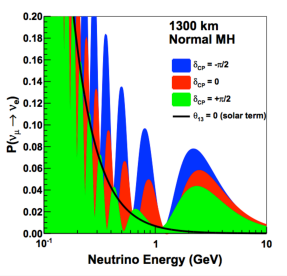
Outline

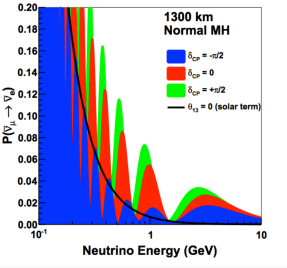
1. Some context
2. Writing a differentiable simulator
3. Results

Some context

Some context with the DUNE experiment



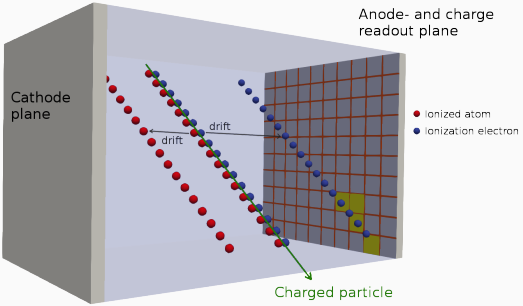


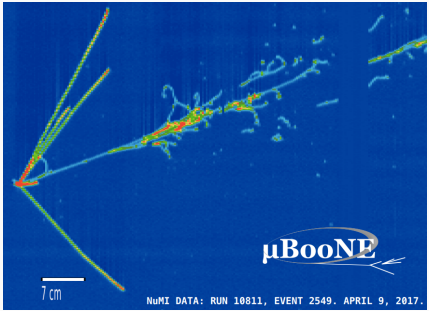


- **DUNE**: **D**eep **U**nderground **N**eutrino **E**xperiment
- Challenging measurement of the oscillation parameters
- Requires **improved resolutions** and **increased mass**

→ Using LArTPC technology

Liquid Argon Time Projection Chambers (LArTPCs)



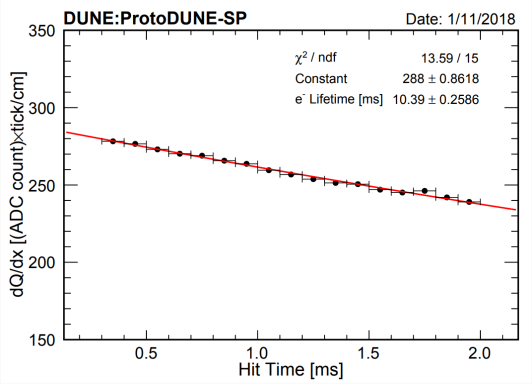


Signal production steps:

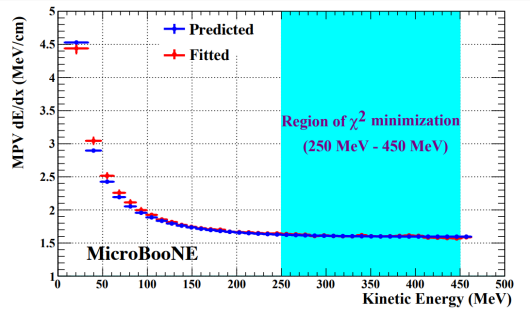
- Argon ionisation
- Ionisation electrons drifted by E field
- Electrons readout on anode plane

- Allows to get **precise 3D picture** of the interaction
- Relies on **multiple physical processes** → importance of calibration

Typical LArTPC calibration



e^- lifetime calibration

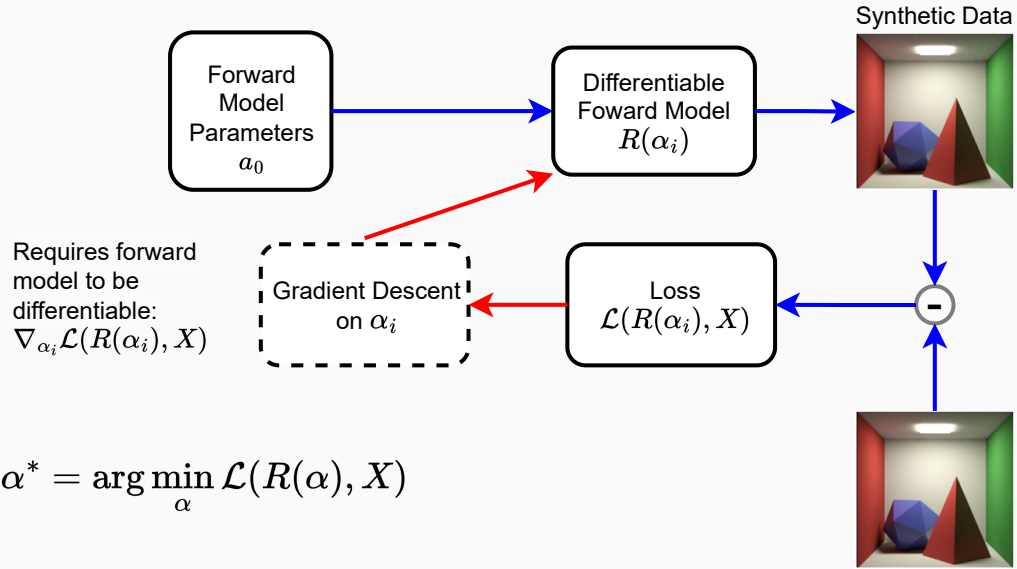


Energy conversion calibration.

Calibration of the different physical parameters are typically done in **different studies**.

→ can be simplified with a differentiable simulator

Using gradient-based optimization



$$\alpha^* = \arg\min_{\alpha} \mathcal{L}(R(\alpha), X)$$

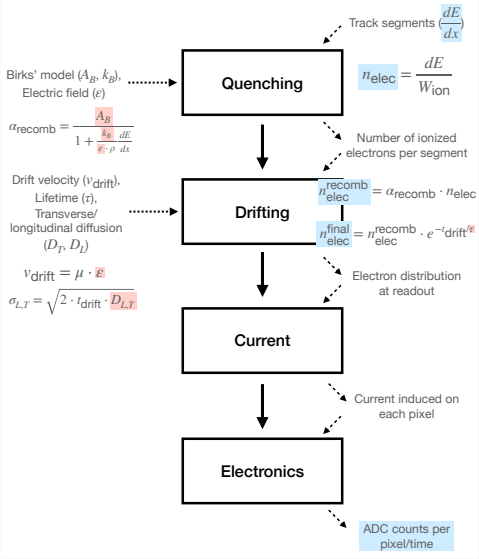
Writing a differentiable simulator

Starting from a non-differentiable LArTPC simulator

Our work: take existing DUNE near-detector simulation (arXiv:2212.09807) and **make it differentiable**.

- Retain physics quality of a tool used collaboration-wide while adding ability to calculate gradient
- Demonstrate the use of this differentiable simulation for **gradient-based calibration**

→ How to do it practice?



Rewriting the simulator

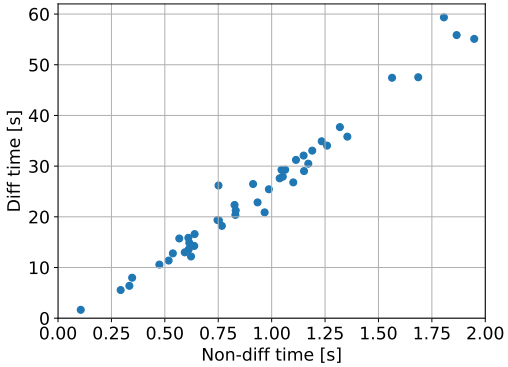
Numba code using **CUDA JIT compiled kernels** → Framework change for diff version:

- Differentiable version rewritten using EagerPy(backend agnostic)/PyTorch, which are based around tensor operations.
- New version rewritten in a **vectorized** way to fit within these frameworks

Performance drawbacks:

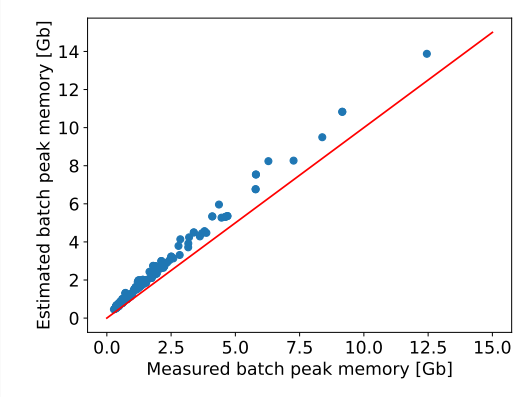
- Use of dense tensors to represent a sparse problem
- Moving from **CUDA JIT compiled dedicated kernel** to a **long chain of generic kernels** (vectorized operations).

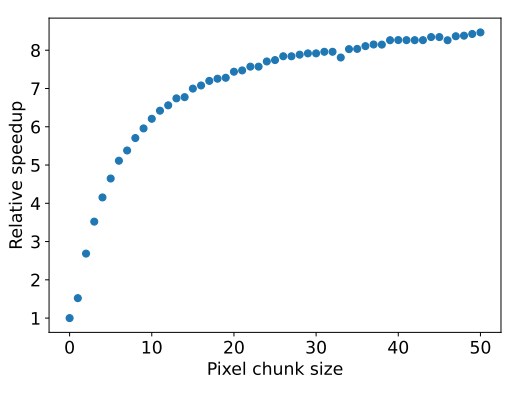
→ also impacting memory usage



Memory challenge

Because of the use of dense tensors, **memory** $\propto \mathbf{\Delta}_z \times \mathbf{cot}\,\theta$. (length in drift direction and angle) $\rightarrow$ introduced **automatic memory estimation** for each batch to estimate best pixel chunk size.



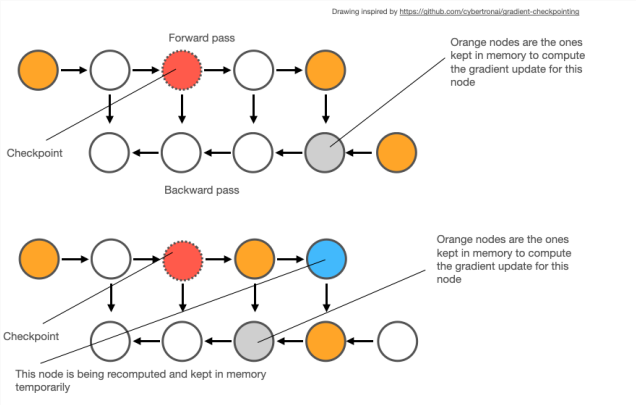


$\rightarrow$ gradient accumulation required by backward pass also saturate the memory

Memory challenge: checkpointing

Reducing the memory used through PyTorch **checkpointing**:

- Gradient accumulation memory intensive due to stored intermediate results
- Trades memory for computation time by recomputing intermediates



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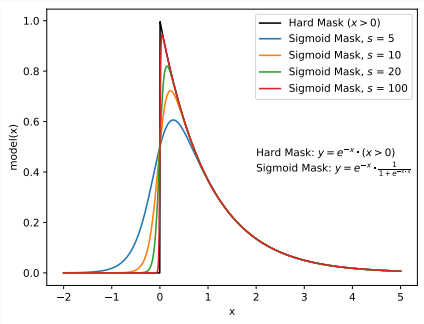
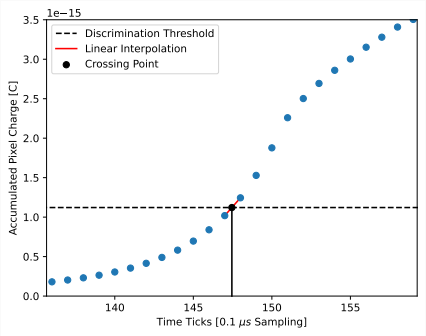
Differentiable relaxations

The base simulation contains **discrete operations** → non-differentiable.

Requires differentiable relaxations to be able to get usable gradients.



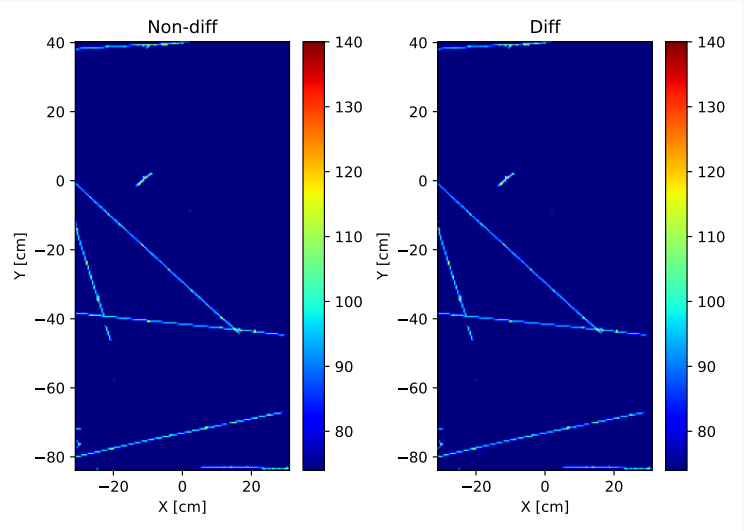


- Cuts (e.g. $x > 0$) → smooth sigmoid threshold
- Integer operations (e.g. floor division) → floating point (e.g. regular division)
- Discrete sampling → interpolation

Checking the result

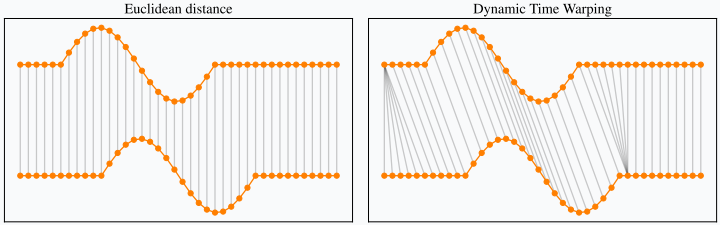
Checking that the **relaxations don't modify the simulator output**.

Average deviation of 0.04 ADC/pixel $\rightarrow$ well below the typical noise level of few ADCs.



Optimization choices: Loss function

Loss function choice is crucial for minimization quality



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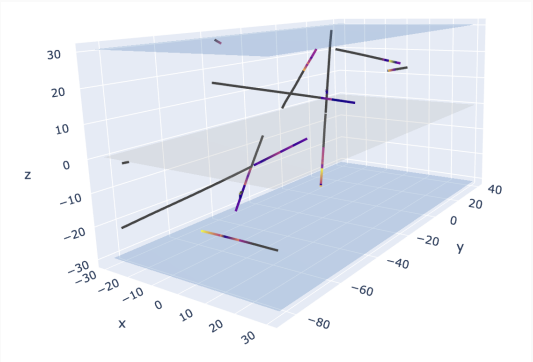
Two main ways of computing the loss:

- Comparison of 3D voxel grids of charges (x, y, t $\rightarrow$ z, q).
  - Difficulty of taking gradients through discrete pixelization.
  - Risk of flat loss if not enough overlap in distributions.
- **Considering the waveforms for each pixel (time sequence) and using Dynamic Time Warping**
  - Using a relaxed SoftDTW version that is differentiable.

Results

Input sample and simulated detector

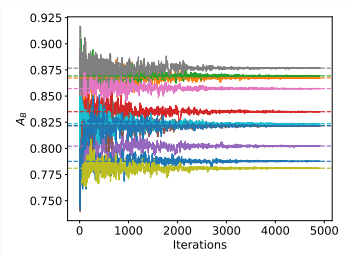
- Input sample consisting of 1 GeV simulated muon tracks
- Second sample of muons, pions and protons (1 GeV to 3 GeV)
- Geometry of a DUNE ND module: 60 cm $\times$ 60 cm $\times$ 120 cm
- Noise model available in simulator but not used.

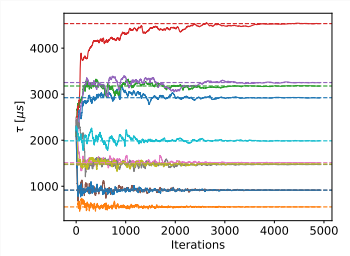


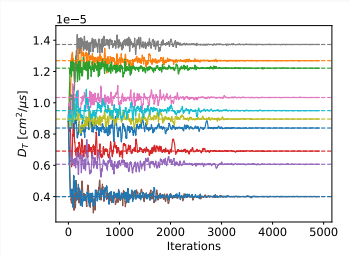
Doing a "closure test" based on simulated data:

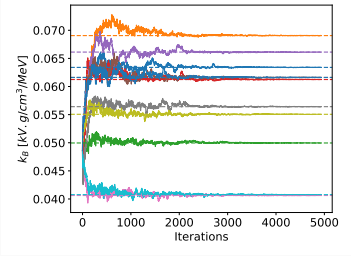
$\rightarrow$ Fit of 6 physical parameters **simulteanously** on simulated data for multiple targets and initial values.

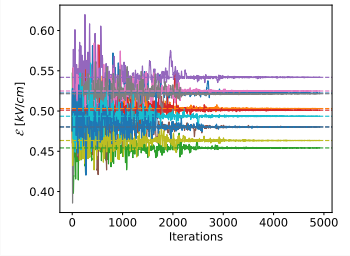
Results

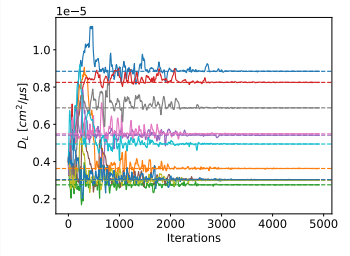






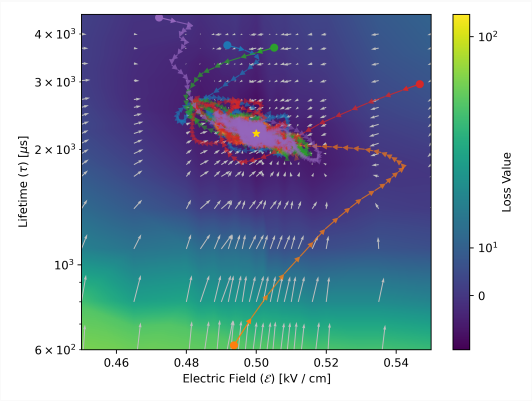




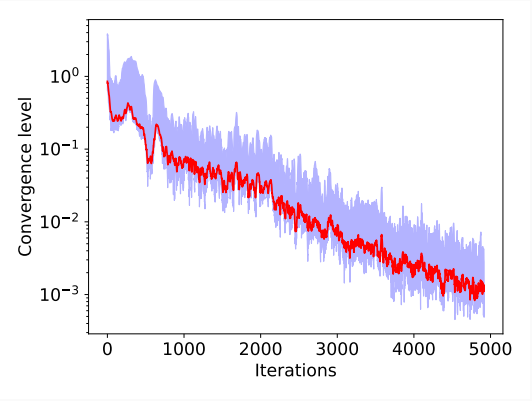


We have **convergence** of the fits for all the parameters.

Results



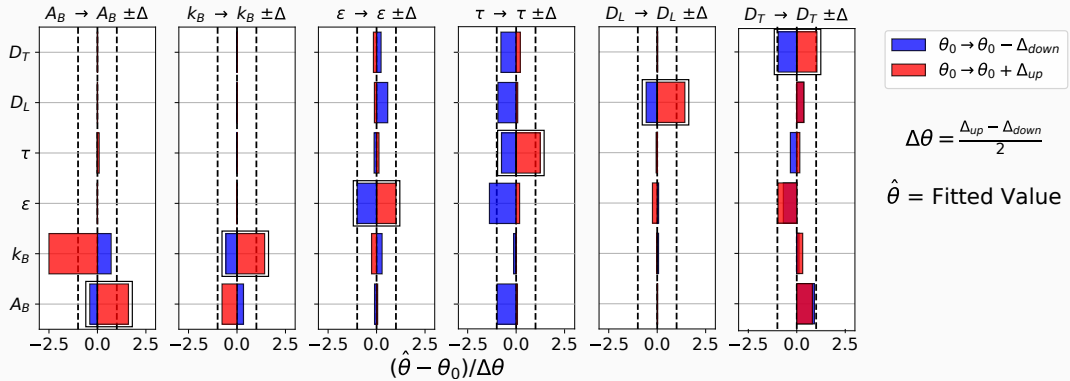
Example of fits "paths" in 2D.



6D simulteanous fit converging under L_∞

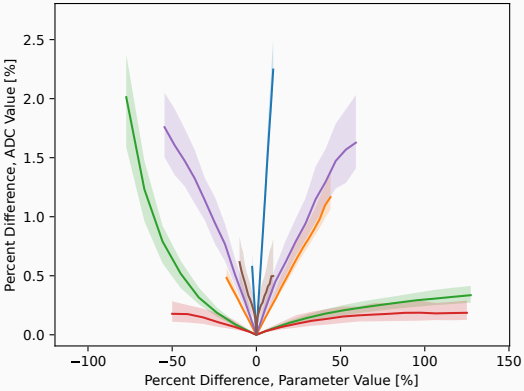
Demonstration of gradient-based calibration on simulation data through a "closure test".

Demonstration of multidimensional fit usefulness

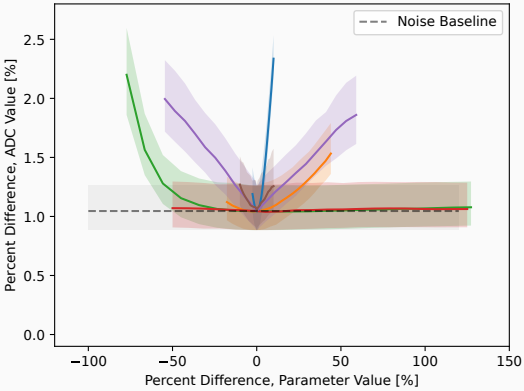


The various physical parameters **are correlated**. Fitting them independently leads to some inaccuracies and biases.

Fit sensitivity

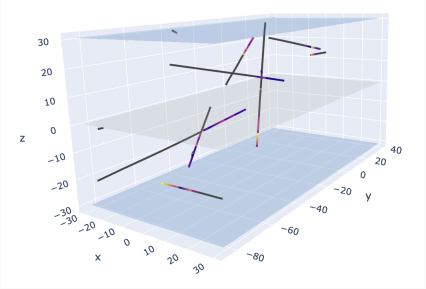


Different sensitivities to the various physical parameters (w.o. noise).



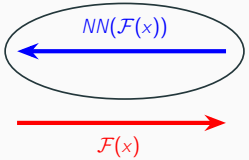
Decrease in sensitivity when considering noise.

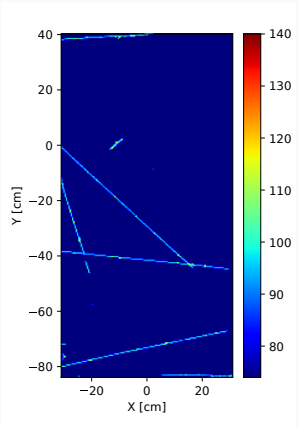
Going further



Energy deposits $\mathrm{d}E/\mathrm{d}x$
(inaccessible in data)

Inverse mapping step to developp





Detector readout

Combining our differentiable simulator with an inverse mapping would allow for direct model constraining, fully data driven: $\mathcal{L}_{CC} = \left(\mathcal{F}(NN(y_{\text{data}})) - y_{\text{data}}\right)^2$

Conclusions

Proof of concept for the calibration of a LArTPC using a differentiable simulator. **Multidimensional fit converging** correctly on simulated data with the differentiable simulator.

Upcoming challenges:

- Applying this framework to real data (DUNE 2x2 ND data)
- Improving the performances (not limiting at the moment)
- Fitting more physical parameters

Going further:

- Extend the framework to inverse problem solving.