Fast Detector Simulation and Detector Design

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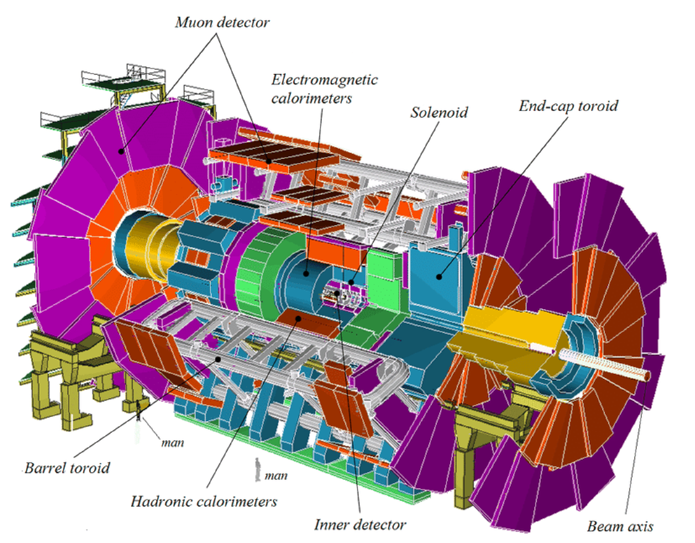
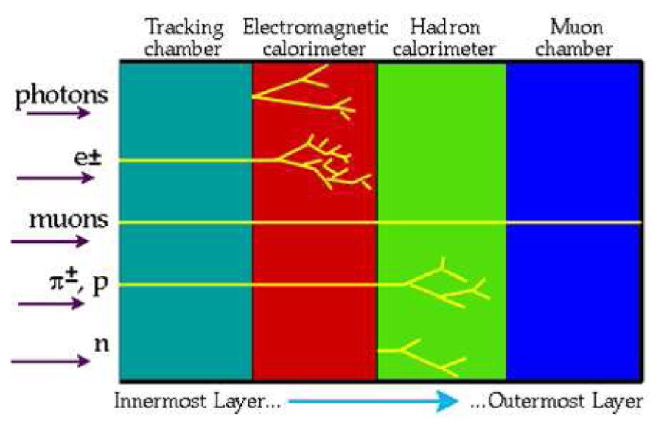
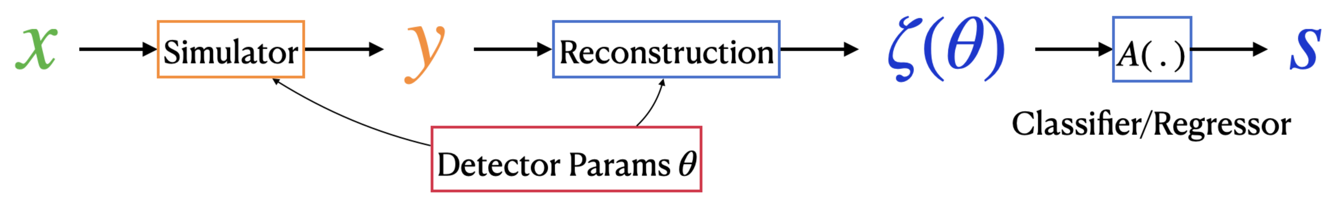
1.Background & Objective: Optimal Detector Design







- Unobserved stochastic input
- PDF : $x \sim f(x)$

- Observed features of the physical process
- Sensor/Simulator readouts
- $y = S(x;\theta) \sim p(y\,|\,x,\theta)$

- Detector/Sensor parameters
- Layout, Material, info. extraction procedures..
- Existing paradigms

- High Level features : $\zeta(\theta) = R\left(y,\theta,\nu(\theta)\right)$
- Low-dim summary statistic : $s = A[\zeta(\theta)]$

$$\hat{\theta} = \arg\min_{\theta} E_{x\sim f, y\sim p(y|x,\theta)}\left[L[A(\zeta), c(\theta)]\right] = \arg\min_{\theta} \int L[A(\zeta), c(\theta)]\,p(y\,|\,x,\theta) f(x)\,dx\,dy$$

- Loss function $L[A(\zeta), c(\theta)]$ constructed to appropriately weight the result of the measurement in terms of its desirable goals [1].
- $c(\theta)$ models the cost of the considered detector layout of parameters θ.
- **Generalised objective** : Can we maximize mutual information between x and y?
  - Reconstruct x from y : use reconstruction performance as loss function.

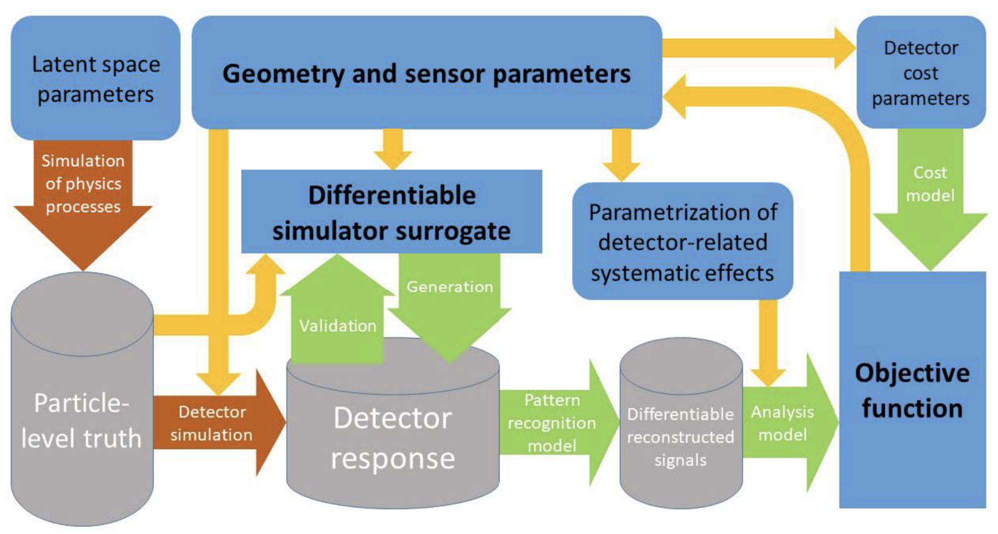
2. Solution Approaches I

- $p(y\,|\,x,\theta)$ not available in closed form and simulator not differentiable w.r.t. θ.
  - Forward simulation to sample from $p(.)$ and approximate:

$$\hat{\theta}_a = \arg\min_{\theta} \frac{1}{n}\sum_{i=1}^{n} L\left[A\left(R\left(y_i\right)\right), c(\theta)\right]$$

  - Differential simulator
  - Surrogates $(y = \hat{S}(z, x, \theta))$:

$$\nabla_\theta(L(\hat{y})) = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta L\left[A\left(R\left(\hat{S}(z_i, x_i, \theta)\right)\right), c(\theta)\right]$$



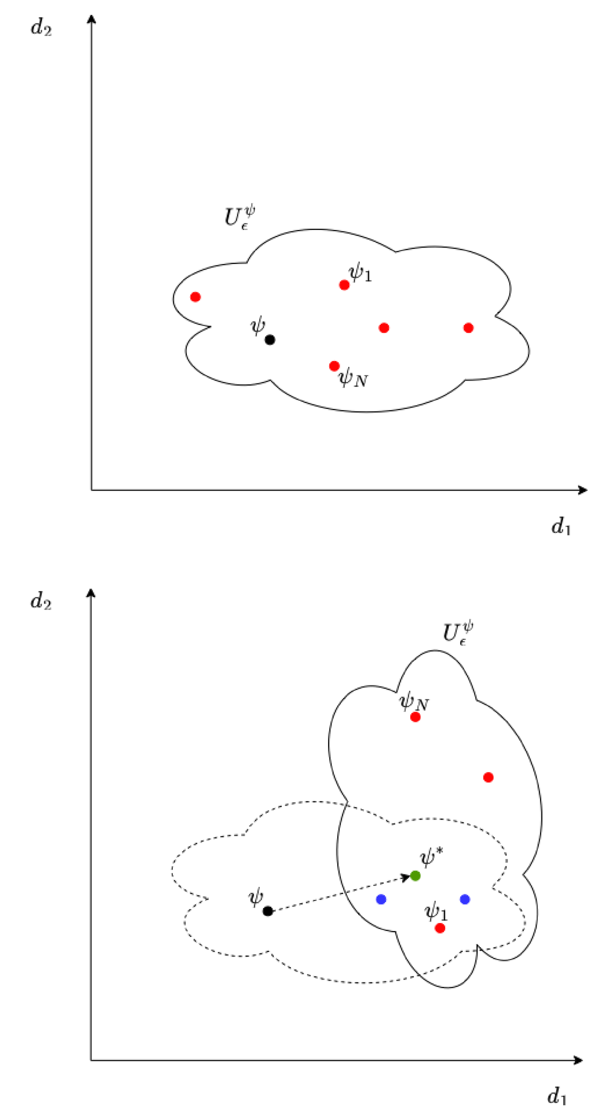
3. Solution Approaches II

- Multiple experimental goals with a single detector/equipment
- **Divide and conquer** : isolate the parameter space θ into different components and optimize them separately for a sub-manifold of possibly sub-optimal solutions.
  - Combine these sub-manifolds to obtain full solution

Algorithm 1 Local Generative Surrogate Optimization (L-GSO) procedure

Require: number N of ψ, number M of x for surrogate training, number K of x for ψ optimization step, trust region U_ϵ, size of the neighborhood ϵ, Euclidean distance d

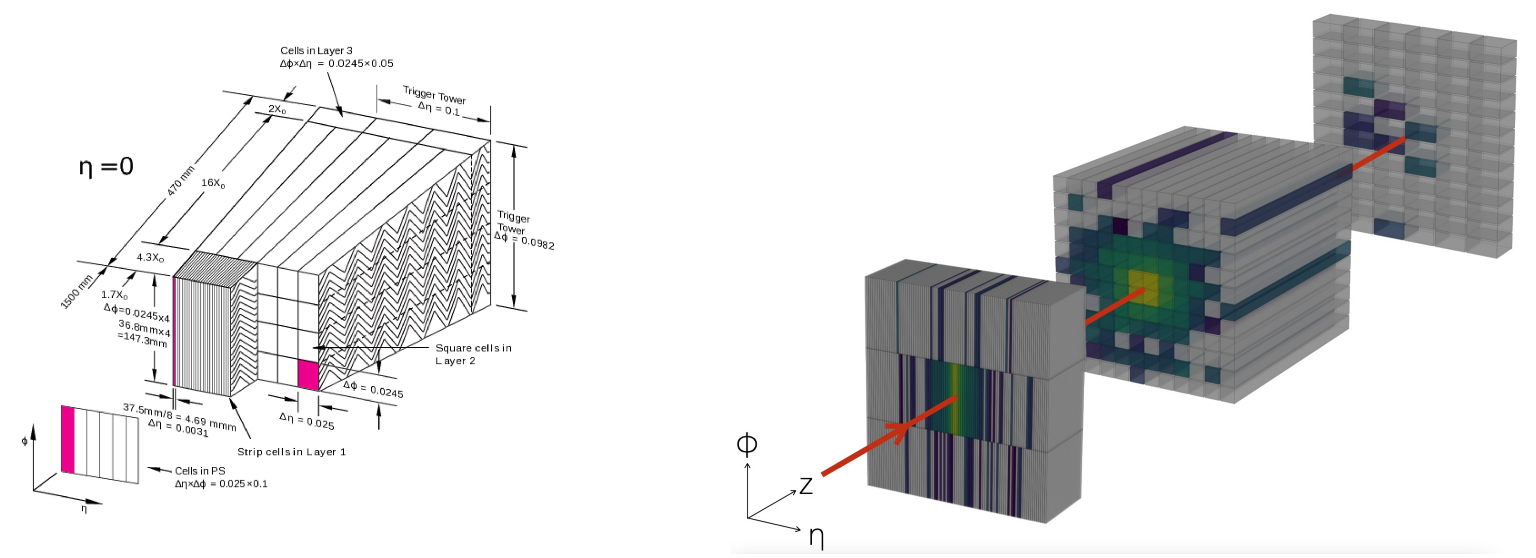
Choose initial parameter ψ
while ψ has not converged **do**
  Sample ψ_i in the region U_ϵ^{ψ}, $i = 1, \ldots, N$
  For each ψ_i, sample inputs $\{x_j^i\}_{j=1}^{M} \sim q(x)$
  Sample $M \times N$ training examples from simulator $y_{ij} = F(x_j^i; \psi_i)$
  Store y_{ij}, x_j^i, ψ_i in history H, $i = 1, \ldots, N$; $j = 1, \ldots, M$
  Extract all y_l, x_l, ψ_l from history H, iff $d(\psi, \psi_l) < \epsilon$
  Train generative surrogate model $S_\theta(z_l, x_l; \psi_l)$, where $z_l \sim \mathcal{N}(0, 1)$
  Fix weights of the surrogate model θ
  Sample $\bar{y}_k = S_\theta(z_k, x_k; \psi), z_k \sim \mathcal{N}(0,1)$, $x_k \sim q(x)$, $k = 1, \ldots, K$
  $\nabla_\psi \mathbb{E}[\mathcal{R}(\bar{y})] \leftarrow \frac{1}{K}\sum_{k=1}^{K} \frac{\partial \mathcal{R}}{\partial \bar{y}_k}\frac{\partial S_\theta(z_k, x_k; \psi)}{\partial \psi}$
  $\psi \leftarrow \mathrm{SGD}(\psi, \nabla_\psi \mathbb{E}[\mathcal{R}(\bar{y})])$
end while



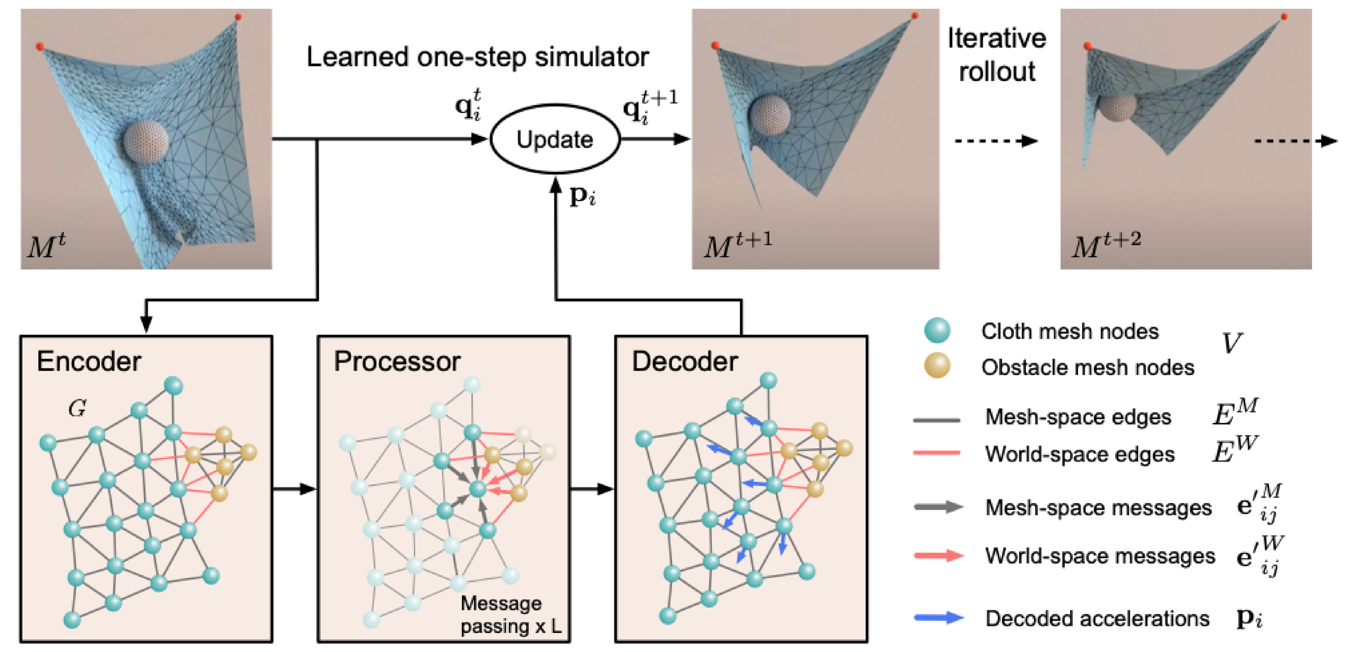
Black-Box Optimization with Local Surrogates [2]

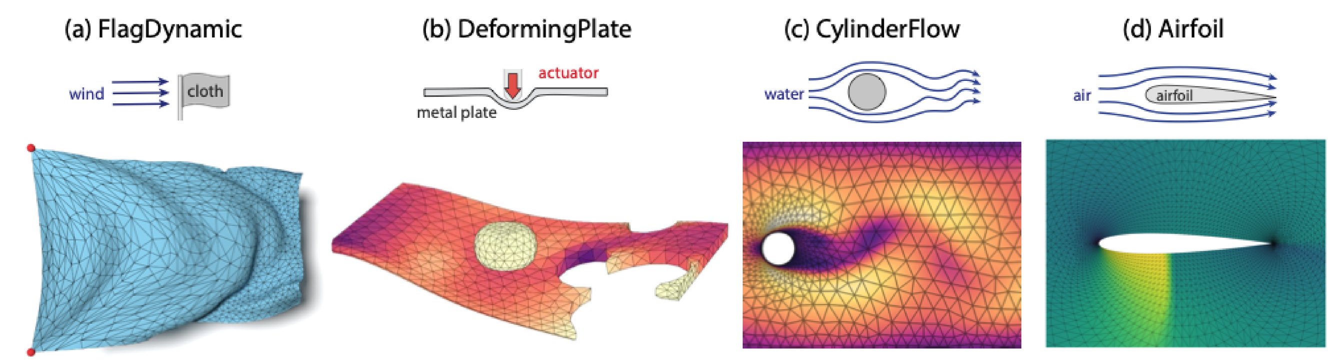
4. Calorimeter Simulation and Optimization

- Simulation helps design detectors during R&D phase and in understanding its response for physics studies and analysis.
- **Geant4** : Physics-based trajectory modelling of particles propagating in material [3].
- **FullSim** framework, iterative and based on Monte-Carlo, initialised with construction of material & geometry, particle types and physics processes.
- Latency bottleneck as $\mathcal{O}(10^{11})$ simulations needed for accurate inference.
- **FastSim** is a trade-off between simulation time and accuracy :
  - Fast simulation hooks in Geant4.
  - Deep generative models : CaloGAN [4], CaloFlow [5], CaloScore [6], etc.
- For optimization of calorimeter design itself → need generative models additionally conditioned on design parameters θ (shape/geometry, material, etc.)

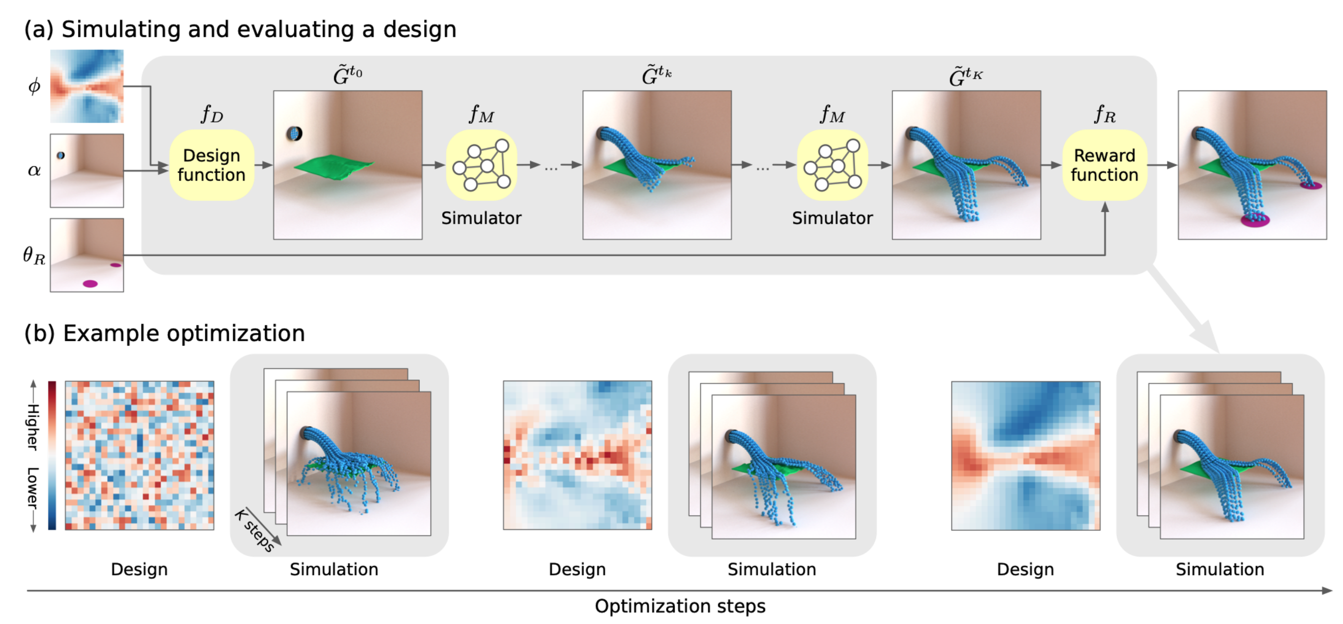


5. Learning General Purpose Physical Simulators





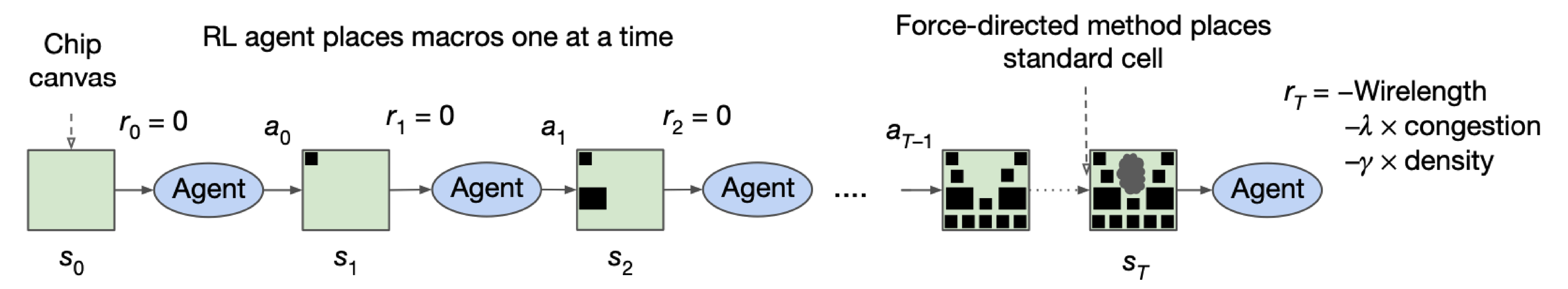
Predicting dynamics of different physical systems, from structural mechanics over cloth to fluid dynamics [7]



Optimizing a physical design [8]

- Goal is to direct a stream of water (shown in blue) into two "pools" (shown in purple) by designing a "landscape" (shown in green) parameterized as a 2D height field

6. Other Examples : Optimal Chip Design



Overview of chip design method [9] and training regimen. In each training iteration, the RL agent places macros one at a time (actions, states and rewards are denoted by a_i, s_i and r_i, respectively). Once all macros are placed, the standard cells are placed using a force-directed method. The intermediate rewards are zero. The reward at the end of each iteration is calculated as a linear combination of the approximate wirelength, congestion and density, and is provided as feedback to the agent to optimize its parameters for the next iteration.

7. References

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