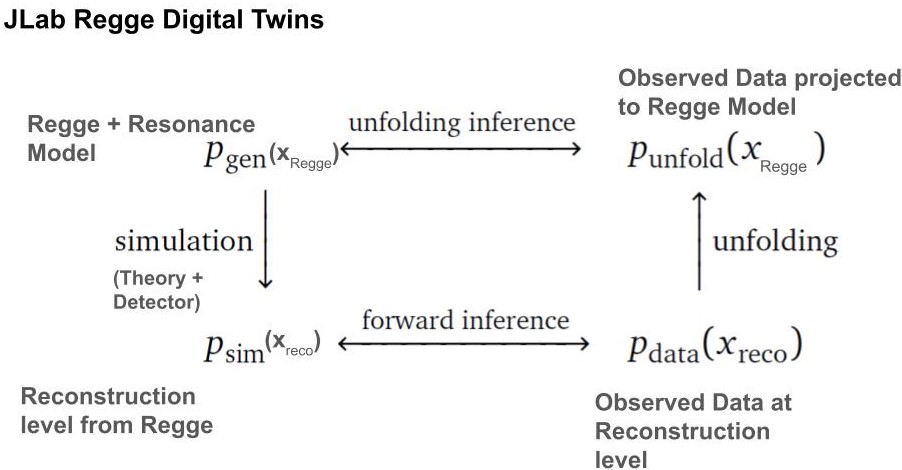
# JLab Regge Digital Twins

*Figure 1: Components of the Jefferson Lab Digital Twin*

This is based on [[1], [2]](https://paperpile.com/c/V7dCTj/XWtX+SDWW) and [2] (see unfolding section). [[3]–[5]](https://paperpile.com/c/V7dCTj/xGwo+S1LK+28x2) are typical of other great papers. These largely look at LHC data with jets and heavy particles. They assume that correct physics is an expansion of parton diagrams with final state phenomenological hadronization. I assume that equally plausible for JLab physics is a Regge plus resonance model with possibilities of ad-hoc backgrounds, absorption, and final state interactions. Let's call this the JLab Regge-Resonance model. The Regge DT (Digital Twin) is an invertible map between observed experimental events and the JLab Regge-Resonance model. It would have parameters such as gluon parameters, Regge Trajectories, and relative fraction of processes. It would produce values and errors with correlations for all JLab Regge-Resonance model parameters.

The experimental data is labeled by xreco and is any consistent experimental level. In principle, one could use data directly from the instruments. Alternatively, the data could be lists of events with reconstructed momenta which is where we would normally look. Finally it could just be any number of selected histograms. In Figure 1, adapted from Figure 1 of [[1]](https://paperpile.com/c/V7dCTj/XWtX), there are two important simulators, as usual in this field. One is the theory simulator from the JLab Regge-Resonance model to pristine lists of particles and properties. The second detector simulator takes pristine particles and folds in detector effects. Note the approach is unchanged if you remove the first simulator. Also, below, I compare theory with experiment, but the approach is the same when comparing two different theories.

The basic technical step is to build an invertble generative AI surrogate to do the map of xRegge  to xreco so that one has a set of 10,000 to 1,000,000 pairs (xRegge, xreco). Note that the notation x is a bit confusing as xRegge and xreco would typically be in totally different spaces (Regge amplitude specification for xRegge or particle specification for xreco. If one was comparing histograms, the x’s would be in the same space. The methods reviewed in [[1]](https://paperpile.com/c/V7dCTj/XWtX) are designed for general (x’s in different spaces) or simpler cases. The mapping to different spaces is naturally done by Encoder-Deoder neural networks sharing a latent space. Note as the simulators involve stochastic choices, one must use a generative AI for a surrogate. Note surrogate is on the left side of Figure 1, and that is inverted on the right-hand side to map experimental data to the theory space. Note results are best formulated as a cloud of points in space as these express all uncertainties from model and detector and stochastic generation. This is a Jefferson Lab digital twin analogous to those for weather [[6]](https://paperpile.com/c/V7dCTj/IBWN).

Earlier papers seem to use invertible normalizing flows but diffusion models are becoming popular. They give better answers than normalizing flows in the well known Kaggle calorimeter challenge.

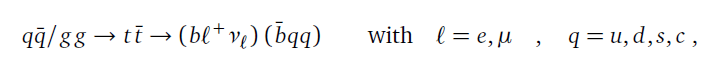
Steps could be

* Start with a theory-to-theory comparison
* Choose simulators
* Generate (xRegge, xreco) pairs
* Generate diffusion model digital twin
* Check you can find details of the second theory
* Apply to real data

The most useful references seem to be “The Landscape of Unfolding with Machine Learning,” from LBL [[1]](https://paperpile.com/c/V7dCTj/XWtX) and “End-To-End Latent Variational Diffusion Models for Inverse Problems in High Energy Physics” [[7], [8]](https://paperpile.com/c/V7dCTj/muuc+fWuQ) from Irvine. The most powerful methods appear to be Direct Diffusion, described by LBL and VLD Latent Variational Diffusion, described by Irvine. LBL, in their Landscape review, actually uses VLD in their most sophisticated analysis from data to theory. LBL uses the RIT VLD software <https://github.com/rxng8/latent-diffusion-jax/tree/main> and this might be a good starting point. I wrote to Nachman for his advice (lead author in LBL group) but no response yet. I personally find VLD a bit clearer to understand as all constraints are present in the loss function which includes the “Evidence lower bound ELBO” term matching the generative distribution functions.

Note reactions considered are pp p to Z plus jet(s) for unfolding detector effects in LBL paper. Here they use many methods, including the diffusion model.

For the unfolding to theory (partons in LBL and Irvine papers, Regge for us), the semi-leptonic top-topbar reaction is used



The results are presented for “theory” to “theory” comparisons. It looks as though we can use their formalism as our Regge reaction is perhaps a little less complex than their parton model. Here LBL (and earlier Irvine) use VLD, although “direct diffusion” should work.

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Background on modern digital twin technology

# 2. Generative AI Approach to Digital Twins

## 2.1 Generative AI for Digital Twins

There are at least three distinct ways that generative AI can enhance digital twins, which we will research in this proposal and show how to integrate them together with mechanism-based simulations. The first use of GenAI is in deep learning surrogates to enhance CC3D simulations, where we leverage our substantial experience in CompuCell3D surrogates [[41], [42]](https://paperpile.com/c/V7dCTj/GGCQu+NwKN5). Surrogates have been very successful in speeding up simulations by developing a deep learning network that feeds the simulation inputs and learns the simulation results [[43]–[48]](https://paperpile.com/c/V7dCTj/LHxIQ+jQird+3R5EM+xR3i6+fptgO+1E5ja). The initial applications tackled deterministic simulations with sophisticated but non-generative AI. Physics-Informed neural networks are also important and relevant [[49]–[52]](https://paperpile.com/c/V7dCTj/EV02A+AcMMc+0ZE4n+9tbjr). In addition, stochastic simulations have also been treated with generative AI networks used to model the Monte Carlo steps. Lattice QCD in theoretical particle physics and experimental calorimeter simulations have been extensively explored [[53]–[56]](https://paperpile.com/c/V7dCTj/OtyhA+sduwf+cN0o2+RGJuN). In spite of these successes, the hybrid situation with many deterministic input parameters combined with stochastic time evolution is not clearly understood. Diffusion models, Normalizing flows, Variational Autoendoers, and GANs have all been investigated for surrogates [[57]](https://paperpile.com/c/V7dCTj/KLr7i). A second generative AI use is for adjusting parameters in a CC3D simulation and comparing simulations with data to find the example that is closest to a particular “patient,” where “patient” is a blinded simulation using a defined mechanistic model and a large number of parameter sets. The challenge here is that the major simulation output is an image (or movie) of a cell field. Often this is done by binning observation (images in our case), but recently generative AI methods [[1], [33]](https://paperpile.com/c/V7dCTj/XWtX+XuMp) (called unfolding or deconvolution, see “Unfolding Section” in [[2]](https://paperpile.com/c/V7dCTj/SDWW)) have been developed to allow individual measurements to be collected together and used without binning. The third area of GenAI use is data assimilation, as described below, which allows one to combine simulations and time-dependent patient-specific observed data in an optimal fashion. Both unfolding and data assimilation AI methods are built around generative AI surrogates and will be essential in this research.

## 2.2 Generative AI for Data Assimilation

Deep Learning and Generative AI have made important progress in understanding data assimilation [[58]](https://paperpile.com/c/V7dCTj/eSSpd). A pioneering paper was [[59]](https://paperpile.com/c/V7dCTj/Heg4K) integrating Deep Learning with Data Assimilation. Assimilation combines simulations and observations to improve forecasting where simulations have uncertainties coming from uncertain boundary conditions, uncertain evolution equations, chaotic points with extreme sensitivity, and stochastic evolution. Kalman filters are a traditional approach, and weather and climate forecasting are traditionally important applications[[60]](https://paperpile.com/c/V7dCTj/6Gyua) . Much of the recent data assimilation progress has come from weather forecasting [[61]–[64]](https://paperpile.com/c/V7dCTj/sUg24+YyHCl+f7sPd+hVY9e) methods in projects such as FourCastNet [[65]–[67]](https://paperpile.com/c/V7dCTj/Oi9Du+l3kqf+A5qVC), AtmoRep [[68]](https://paperpile.com/c/V7dCTj/GQh8A), GraphCast, Fuxi-DA [[69]](https://paperpile.com/c/V7dCTj/1U4CX), NeuralGCM [[70]](https://paperpile.com/c/V7dCTj/BMAbW), FengWu-GHR [[71]](https://paperpile.com/c/V7dCTj/dR6LM), NowcastNet [[72]](https://paperpile.com/c/V7dCTj/BHej4), MetNet-3 [[73]–[75]](https://paperpile.com/c/V7dCTj/0qwnq+YKHyK+mZ4tO) and GraphCast [[73], [76]–[82]](https://paperpile.com/c/V7dCTj/0qwnq+O1mQw+v8l3D+q9wEs+wOvTV+222vx+QWQF1+qAvBk) (Google), Pangu [[83]–[85]](https://paperpile.com/c/V7dCTj/aXdIt+R8zNG+uErTP) (Huawei), Corrformer [[86]](https://paperpile.com/c/V7dCTj/nWcy6), KARINA [[87]](https://paperpile.com/c/V7dCTj/F3ftz), Graph Neural Networks for weather [[88]](https://paperpile.com/c/V7dCTj/pXfCL), DiffDA [[6]](https://paperpile.com/c/V7dCTj/IBWN), and CorrDiff/Earth-2 [[89]–[94]](https://paperpile.com/c/V7dCTj/lZ5BC+y243a+N0abj+t053g+RxHvn+K9WUe) (NVIDIA). The major involvement of (inter)national meteorological services and Industry has accelerated progress. There is related progress in Foundation models for this and related fields such as ClimaX [[95], [96]](https://paperpile.com/c/V7dCTj/exCTe+ushs0) from Microsoft (extended by ORBIT: Oak Ridge Base Foundation Model for Earth System Predictability [[97]](https://paperpile.com/c/V7dCTj/YNG88)) and Prithvi (IBM and NASA [[98]–[100]](https://paperpile.com/c/V7dCTj/niDj7+eTl5r+gnaE1)). The GenAI methods can naturally include all the uncertainties listed above, and it can represent the system as an ensemble where the variation in model properties is the uncertainty at any one time. These grow or decrease as evolves the simulation or conversely constrains with an assimilation. [[6]](https://paperpile.com/c/V7dCTj/IBWN) used 16 replicas in a weather ensemble. We will research the needed number in our case, expecting 1000-10,000 replicas to be appropriate. Note that evolving these replicas involves computer system workflow technologies with which we are very experienced [[101]–[103]](https://paperpile.com/c/V7dCTj/McZ0G+D9clg+Z03dr). The application of GenAI-based data assimilation will probe new research issues reflecting differences between weather and virtual tissue domains. Some of these differences include the need to use significant time series in Virtual Tissues, whereas, in many weather forecast studies, the basic step is often just a single forward prediction from time t to time t plus 6 hours. The personalization step in Virtual Tissues is challenging, whereas in the weather case, one already has, for any region, good initial conditions, a history of the recent states of the system, and well-understood physics of evolution equations. We will explore the idea of differentiable simulations [[104], [105]](https://paperpile.com/c/V7dCTj/Qg4eF+IM8RN) already applied to the weather case so that we can simultaneously optimize the AI, the mechanistic model parameters, and the user-defined metrics of simulation outcomes.

In addition, we will compare the machine-derived image descriptors (such as latent space descriptions) versus user-defined metrics and, finally, combine the sets of descriptors. The machine-derived metrics have the advantage of being “naive” (unbiased) to the details of the simulation, whereas the user-defined metrics have the advantage of interpretability by a human but include human bias. Recently, there has been intense interest in Foundation models [[106]–[110]](https://paperpile.com/c/V7dCTj/0XfYw+RI2e3+qNUY1+QGRXS+rh8Ok) with pre-training on large datasets and fine-tuning for particular tasks. We will evaluate both Foundation model approaches and those using single training cycles. Contact with outside communities (MLCommons [[111]](https://paperpile.com/c/V7dCTj/ASxDN), the AI Alliance [[112]](https://paperpile.com/c/V7dCTj/WiosD), and the Trillion Parameter Consortium [[113]](https://paperpile.com/c/V7dCTj/VmBUi)]) will allow us to keep abreast of the latest developments there.

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