

## Enforcing Imprecise Constraints on Generative Adversarial Networks for Emulating Physical Systems

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**Abstract.** Generative adversarial networks (GANs) were initially proposed to generate images by learning from a large number of samples. Recently, GANs have been used to emulate complex physical systems such as turbulent flows. However, a critical question must be answered before GANs can be considered trusted emulators for physical systems: do GANs-generated samples conform to the various physical constraints? These include both deterministic constraints (e.g., conservation laws) and statistical constraints (e.g., energy spectrum of turbulent flows). The latter have been studied in a companion paper (Wu et al., Enforcing statistical constraints in generative adversarial networks for modeling chaotic dynamical systems. *Journal of Computational Physics*. 406, 109209, 2020). In the present work, we enforce deterministic yet imprecise constraints on GANs by incorporating them into the loss function of the generator. We evaluate the performance of physics-constrained GANs on two representative tasks with geometrical constraints (generating points on circles) and differential constraints (generating divergence-free flow velocity fields), respectively. In both cases, the constrained GANs produced samples that conform to the underlying constraints rather accurately, even though the constraints are only enforced up to a specified interval. More importantly, the imposed constraints significantly accelerate the convergence and improve the robustness in the training, indicating that they serve as a physics-based regularization. These improvements are noteworthy, as the convergence and robustness are two well-known obstacles in the training of GANs.

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# 1 Introduction

## 1.1 Physical applications of GANs: progress and challenges

Machine learning and particularly deep learning has achieved significant success in a wide range of commercial domain applications such as image recognition, audio recognition, and natural language processing [1–5]. In recent years, machine learning has been widely adopted in scientific applications, leading to an emerging field referred to as *scientific machine learning*. Example scientific applications of machine learning include augmenting or constructing data-driven turbulence models [6–8], generating realistic animations of flows [9–12] discovering or solving differential equations [13–19].

Recently, generative adversarial networks (GANs) [20] emerged as a promising model in machine learning. GANs construct mappings from a generic (e.g., uniform or Gaussian) probability distribution to the data distribution. Once trained, such models can generate new samples that are not in the training database but conform to the data distribution. As the training only uses unlabeled data, generative models belong to unsupervised learning. GANs have shown promises in many scientific applications from synthesizing CT-scan images of rocks [21, 22] to generating flow fields [12, 23, 24] or solutions of ordinary, partial or stochastic differential equations [25–27]. The successful applications to physics prompt a critical question on the capability of GANs: do they generate samples that conform to the underlying physical constraints? These constraints are implicitly embedded in the training data to certain accuracy, because the data are obtained either by solving the equations that *reflect* these constraints or by directly observing the physical system that *obey* such constraints. However, the constraints are not explicitly encoded in the GANs. In the above-mentioned applications, the generated output are physical fields that often reside in high-dimensional spaces. This is in contrast to supervised learning, where the output are multi-class labels or low-dimensional scalar and vectors (e.g., the permeability or velocity at a point). Taking the GANs based PDE-emulator for example [26], the output temperature field discretized on a mesh of  $100 \times 100$  grid points has a dimension of  $10^4$ . Nevertheless, the physical laws expressed in the form of PDEs place heavy constraints on the admissible solutions. For example, velocity fields of fluid flows must be divergence-free due to mass conservation; temperature fields are typically smooth due to the Laplace operator in the governing equation. Such constraints dictated that admissible (i.e., physical and realistic) solutions must lie on a low-dimensional manifold embedded in a high-dimensional space. Therefore, it is imperative to ensure the constraint-respecting properties of GANs before using them as trusted emulators for physical systems.

Fortunately, it has been theoretically proven that GANs are capable of preserving all the constraints and statistics of the training data, up to the expressive capability of the generator and discriminator neural networks, if the global optimum is achieved in the training [20]. However, it is also well-known that traditional GANs has difficulty in convergence and lack robustness in the training [28, 29]. Consequently, numerous efforts