# A Wasserstein GAN with Gradient Penalty for 3D Porous Media Generation.

<table>
<thead>
<tr>
<th>Item Type</th>
<th>Conference Paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>Authors</td>
<td>Corrales Guerrero, Miguel Angel; Izzatullah, Muhammad; Hoteit, Hussein; Ravasi, Matteo</td>
</tr>
<tr>
<td>Eprint version</td>
<td>Post-print</td>
</tr>
<tr>
<td>DOI</td>
<td>10.3997/2214-4609.2022616005</td>
</tr>
<tr>
<td>Publisher</td>
<td>European Association of Geoscientists &amp; Engineers</td>
</tr>
<tr>
<td>Rights</td>
<td>This is an accepted manuscript version of a paper before final publisher editing and formatting. Archived with thanks to European Association of Geoscientists &amp; Engineers.</td>
</tr>
<tr>
<td>Download date</td>
<td>2023-11-01 06:53:40</td>
</tr>
<tr>
<td>Link to Item</td>
<td><a href="http://hdl.handle.net/10754/685625">http://hdl.handle.net/10754/685625</a></td>
</tr>
</tbody>
</table>
Summary

Linking the pore-scale and reservoir-scale subsurface fluid flow remains an open challenge in areas such as oil recovery and Carbon Capture and Storage (CCS). One of the main factors hindering our knowledge of such a process is the scarcity of physical samples from geological areas of interest. One way to tackle this issue is by creating accurate, digital representations of the available rock samples to perform numerical fluid flow simulations. Recent advancements in Machine Learning and Deep Generative Modeling open up a new promising avenue for generating realistic digital rock samples at low cost. This is particularly the case for Generative Adversarial Networks (GANs) due to their ability to learn complex high-dimensional distributions and produce high-quality samples. The present study introduces a novel Wasserstein GAN with gradient penalty (WGAN-GP) to generate 3D high-quality porous media samples. Moreover, a comprehensive set of evaluation metrics inspired by the geometry and topology of the structure and the fluid flow properties is established to assess the quality of the generative process.
Introduction

Understanding the fluid flow at the pore scale requires accurate characterization of the host rock. Unfortunately, the cost of extracting samples from the reservoir of interest coupled with the variability of rock properties make such a task arduous and economically expensive. Moreover, when rock samples are available, they are prone to damage when used in laboratory experiments. Digital Rock Reconstruction, on the other hand, intends to image rock samples by means of computer tomography (CT) and process them to obtain a 2D or 3D binary representation of their pore structure. Later, numerical simulations can be carried out using the digital structure to evaluate the fluid flow phenomena and interpret the controlling properties of the rock. In the past, multiple-point statistics has been used to generate rock representations aligned with their in-situ properties (Okabe and Blunt, 2005). Such techniques are well-established and considered standard practice to overcome the lack of physical samples.

In the last decade, advancements in Deep Generative Modeling have brought new and more robust alternatives to directly sample from complex distributions purely represented by a set of training data (Goodfellow et al., 2014). Generative Adversarial Networks (GANs) represent one such kind of generative model, which has been recently used by Mosser et al. (2017) to obtain replicas of different porous media. Nonetheless, since the introduction of GANs, new improvements and techniques have been established in the computer vision area that could also be beneficial in accelerating and improving the generation process of porous media.

This work introduces a novel Wasserstein GAN with Gradient Penalty (WGAN-GP) algorithm to produce 3D realistic porous media samples, which avoids an expensive training stage. Also, it suggests a new way to perform data augmentation based on Representative Elementary Volume (REV). Moreover, it assesses if including rock physics constraints during the training process could improve the quality of the generative model. Lastly, several metrics are proposed to specifically assess the performance of generative models of porous media.

Theory

Generative Adversarial Networks (GANs)

The main objective of GANs is to produce samples from high-dimensional data distributions. Commonly, a GAN is composed of two independent networks: a generator (G) and a discriminator (D), also known as critic. The generator is tasked to produce samples from a latent space representation whose distribution \( p_g \) mimics the training data (\( p_d \)). On the other hand, the critic aims to distinguish between the real (\( x \)) and generated (\( \hat{x} \)) samples. In the original GAN formulation of Goodfellow et al. (2014), the discriminator’s loss was built upon the idea that the generator should learn to approximate the data distribution through the Jansen-Shannon divergence. Unfortunately, this formulation suffers from the vanishing gradient issue due to the use of a binary cross entropy loss that is easily saturated, thus hindering the generator to be updated further. This formulation also shows a mode-seeking behaviour, which leads to the mode-collapse phenomenon. Several strategies have been devised in order to overcome these limitations, such as reformulating the GAN loss function in terms of the Wasserstein distance (WGAN) (Arjovsky et al., 2017) and introducing a Lipschitz continuity gradient norm penalty (WGAN-GP) (Gulrajani et al., 2017). See Table 1 for the loss functions of the different formulations.

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Discriminator Loss ((L_D))</th>
<th>Generator Loss ((L_G))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original</td>
<td>(-E_{x \sim p_d} \log(D(x)) - E_{\hat{x} \sim p_g} \log(1 - D(\hat{x})))</td>
<td>(E_{\hat{x} \sim p_g} \log(1 - D(\hat{x})))</td>
</tr>
<tr>
<td>Non-Saturating</td>
<td>(-E_{x \sim p_d} \log(D(x)) + E_{\hat{x} \sim p_g} \log(D(\hat{x})))</td>
<td>(-E_{\hat{x} \sim p_g} \log(D(\hat{x})))</td>
</tr>
<tr>
<td>WGAN-GP</td>
<td>(-E_{x \sim p_d} [D(x)] + E_{\hat{x} \sim p_g}[D(\hat{x})] + \lambda E_{\hat{x} \sim p_g} \left(\left|\nabla D(\alpha x + (1 - \alpha)\hat{x})\right|_2 - 1\right)^2)</td>
<td>(-E_{\hat{x} \sim p_g} [D(\hat{x})])</td>
</tr>
</tbody>
</table>

Table 1 Summary of different GAN formulations introduced to improve the network’s training process. Here, \(E_{x \sim p}\) denotes the samples expectation on distribution \(p\) (usually computed as sample mean over the true or generated samples), and \(\alpha\) is the sample interpolation coefficient for the gradient penalty computation in WGAN-GP.

Evaluation metrics

A trained GAN requires a quantitative evaluation of its sampling capabilities. A metric commonly used to evaluate the quality and variety of the generated samples is the Frechet Inception Distance (FID), which computes the similarity between the real (\( x \)) and generated (\( \hat{x} \)) samples. However, the Incep-
Two-point statistics are routinely used to characterize the structure of porous media: they represent the probability that two points within a $d$-dimensional space $\mathbb{R}^d$ and separated by a lag vector $r$ occur in the same phase (grains or pore space). Formally, two-point correlation is expressed as $\delta_2^{(i)}(r) = \text{P}(x \in V_i, x + r \in V_i)$ for $x, r \in \mathbb{R}^d$, where $x$ is an index referring to a pixel’s location in the porous media’s binary representation. Assuming the medium to be homogeneous and isotropic, two-point correlation can be computed using the fact that the auto-correlation function is the inverse Fourier Transform of the power spectrum density (Gostick et al., 2019). Similarly, the morphology of the complex structure of porous media could be described by the Minkowski functionals. These functionals characterize the rock structure based on their geometry and topology. The structure is characterized by a linear combination of $d + 1$ independent parameters where $d$ represents the dimension of the structure. Considering a 3D porous medium $(X)$ with a smooth boundary $(\partial X)$, the Minkowski functionals are presented in Table 2. They are related to porosity, surface area, mean curvature, and the Euler characteristic (Boelens and Tchelepi, 2021). For example, porosity can be easily computed on the 3D binary representation as the ratio of pore volume to the total volume (number of voxels representing the pore phase over the total number of voxels).

<table>
<thead>
<tr>
<th>Porosity</th>
<th>Surface Area</th>
<th>Mean curvature</th>
<th>Euler characteristic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_0(X) = \int_X dv$</td>
<td>$M_1(X) = \frac{1}{8} \int_{\partial x} ds$</td>
<td>$M_2(X) = \frac{1}{2\pi^2} \int_{\partial x} \frac{1}{r_1} \frac{1}{r_2} ds$</td>
<td>$M_3(X) = \frac{3}{4\pi^2} \int_{\partial x} \frac{1}{r_1 r_2 r_3} ds$</td>
</tr>
</tbody>
</table>

Table 2 Minkowski functionals for 3D objects. Here, $ds$ is the surface element, $R$ radius of the local curvature, $dv$ the volume element, $R_1$ and $R_2$ the principal radii of curvature of the surface element.

Finally, a rock is also characterized in terms of its dynamics properties such as permeability, which is defined as the ability of the rock to transmit fluids. The permeability of digital rocks can be computed by solving the steady-state Stokes equation for incompressible flow under gravity with no-slip boundary conditions. Once the velocities are obtained, Darcy’s Law is applied to determine the absolute permeability value (Wang and Sun, 2016).

**RockGAN**

In this section, we present RockGAN, a novel GAN architecture designed to create 3D realistic porous media samples. Its generator consists of a set of four transpose convolutional blocks followed by Gaussian Error Linear Unit (GELU) activation functions, except for the last layer that uses a sigmoid activation to produce binary pore-scale samples. The generator grows progressively starting from a latent random noise representation of $16 \times 16 \times 16$, and doubling its size every layer to reach the final dimensions of $128 \times 128 \times 128$. Similarly, the discriminator is designed to follow a mirror representation (from high to low resolution). It consists of six convolutional blocks followed by Instance Normalization and LeakyReLU activation function. The networks details are illustrated in Figure 1c.

RockGAN is trained using the loss function of WGAN-GP in table 1. Moreover, a rock physics soft-constraint in the loss function based on the porosity measured from each generated sample could improve the training and lead to improved quality of the generated rock samples. This is mathematically expressed as the mean square error (MSE) between the porosity of each generated sample and the mean porosity of the real dataset. Ideally, such a constraint attempts to reduce the distribution’s standard deviation and align the samples closer to the mean property values (i.e., porosity). This extra loss term is added here to the both the generator and discriminator. We call this network C-RockGAN.

**Numerical examples**

A 3D sample of Berea sandstone, composed of 400 voxels with voxel size equal to 3 micrometers (Mosser et al., 2017), is used to test the proposed RockGAN and C-RockGAN. A Representative Elementary Volume (REV) analysis is initially performed to extract a meaningful number of sub-volumes.
from the original sample and create the training dataset. The REV evaluation is carried out in this case by analysing porosity and permeability: Figure 1b illustrates the properties distribution at the different sub-volume sizes. Porosity and permeability are computed at different sub-volumes sizes extracted from the original sample. Our main criterion to define the optimum size is based on a trade-off between i) identifying a size that leads to a narrow distribution whose mean is close to that of the original sample and, ii) maintaining the required computational resources to an acceptable level. Based on this, we select a sub-volume size for extraction equal to 128 voxels as it preserves the average rock characteristics of the original 3D sample and guarantees a relatively good resolution at a reasonable computational cost. As a result of this choice, the training dataset is composed of 1024 extracted volumes.

Two networks are trained using the original, and the rock-physics constrained WGAN-GP loss functions, respectively. Both networks are trained for 100 epochs. Their performance is compared by evaluating the mean value of the Minkowski functionals and the permeability, and also the MSE of the two-point statistics of the samples generated at each epoch. The hyper-parameters are kept equal, aiming only to assess if the extra term in the loss function provides any benefit to the training process. Figure 2a shows the training progress based on the established metrics. Here, we present some insights: 1) irrespective of the formulations, the network seems to be able to learn high-level statistics and generate a realistic representation of the Berea dataset (See Figure 2a for metrics and Figure 2b for the visual evolution on random 2D profiles at different epochs, and figure 2c for comparison with true 2D profiles); 2) There is low significant influence of the porosity constraint introduced on the generator and discriminator. Both architectures follow a similar trend along the media of the Minkowski functionals computed (See Figure 2a showing only porosity and surface as an example), permeability, and MSE of the two-point statistics. Similar quality generation evolution results in visual representation in 2b along the training. The relatively less significant influence of the rock-physics constraint could be attributed to the fact that the architecture of the network is robust enough to learn the Berea representation. Also, a suitable metric that compares the distribution between the generated and real dataset is needed apart from the physical characteristics of the rock. A fair comparison could be achieved using the FID score. Based on the qualitative evaluation of 2D profiles and quantitative metrics, around epoch 80, the best representation of the medium is achieved (see 3D results compared to the original dataset in Figure 2c).

Conclusions

We have presented a robust and powerful WGAN-GP network for the unconditional generation of 3D rock samples. Its success is determined based on the fact that generated samples honor physical metrics such as the Minkowski functionals, permeability, two-point statistics, and that high-quality samples are produced already at a highly reduced number of epochs. In addition, RockGAN can capture both the small and big pore throats and their connectivity (visually examined). This work also emphasizes the
importance of carrying out a REV analysis before performing data augmentation. Extracting a sub-volume size not representative of the original rock properties implies a generation of samples from a different medium compared to that of interest. We finally note that adding a porosity constraint to the loss function does not improve the quality of RockGAN. More rock types and different physical constrains (e.g., surface area) will be tested in future to assess the possible added value of physical constraint in the training process.

![Figure 2](image_url)  
**Figure 2** a) Metrics evolution over epochs. Porosity is the only parameter constrained C-RockGAN. b) 2D profiles evolution for the two GANs investigated (white=grain, black=pore). c) 3D visual comparison between two generated samples after epoch 80 and two sub-volumes of the Berea training dataset.

Acknowledgements

The authors thank King Abdullah University of Science and Technology (KAUST) for supporting this research. We also thank Prof. Mohamed Elhoseiny and Prof. Shuyu Sun for their insightful comments on Generative Models and fluid flow at the pore scale, respectively. For computing resources, this study used The KAUST Supercomputing Laboratory. The code repository of this work can be found at https://github.com/DIG-Kaust/RockGAN.

References


