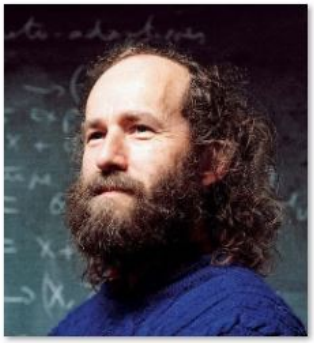
Written on 21 June 2021 15 minutes of reading

News

Fundamental Research



When Machine Learning reached maturity in the 2010s, with the advent of deep learning, the scientific landscape, across all fields, was profoundly altered, marked by the availability of mass data.

And the impact is now being observed in the field of numerical simulation. But Deep Learning is more than a highly powerful regression method and should also be considered as the nucleus of Differentiable Programing[1]. The enlightened deployment of this approach, in conjunction with traditional methods used in the target fields, paves the way to rapid scientific progress.

Today, the fact is that complex physical, mechanical, chemical, biological and artificial systems are confronted with massive quantities of data,

- be it input data, generated by cheap sensors, which can be found everywhere;
- or output data, generated by numerical simulations of mechanistic models, which are now

mature in many fields.

We are thus able to take advantage of both ends of the chain: from the integration of real-world data into existing ODE and PDE[2] mechanistic models through to the derivation of entirely new models, directly from real data, respecting the known properties of the system under consideration[3].

This special issue illustrates how IFPEN is taking advantage of this revolution, combining its existing expertise with creativity to develop innovative solutions.

Marc Schoenauer, INRIA-Saclay
Member of IFPEN's Scientific Board

1- Combining Machine Learning and numerical optimization
2- Respectively: Ordinary Differential Equation and Partial Differential Equation
3- For example, the conservation of mass, energy dissipation, geometric invariance, etc.

LES BRÈVES

Numerical simulations are now widely employed in the industrial world to help design systems and predict complex phenomena. Reactive flow simulation, for example, is important for numerous applications, such as vehicle and aircraft propulsion and processes in the chemicals industry.

Reactive flows involve mixtures of chemical constituents and compounds that react with each other resulting in, depending on the nature of these reactions, an evolution of species over periods of time that can vary widely. Describing the temporal evolution of these species within the flow requires the use of advanced numerical methods - i.e., costly calculation times - and solving these equations accounts for a significant part of the total simulation time for a system.

The use of learning methods to speed up chemical kinetics calculations is an approach that has recently gained in popularity. When calculating an industrial system, the idea is to replace traditional resolution algorithms with an equivalent model, derived from a learning process, that can be evaluated more quickly. This model is generated by optimizing a set of parameters from a database of exact, previously simulated solutions.

To do this, researchers at IFPEN used neural networks, due to their capacity to reproduce the evolution of chemical species. The research focused on two areas.

- The first compared different neural network structures to predict the evolutions of chemical species. Standard networks were compared to so-called “recurrent” neural networks, making it possible to establish predictions taking into account a set of past values, rather than a single value.

- The second focused on physicochemical constraints, in particular the need to respect the conservation of mass for each element present in the mixture, something that is not guaranteed with neural networks traditionally used.

The methodology deployed was evaluated for the homogeneous combustion of hydrogen. In this situation, since the mass fractions do not vary in space, numerical resolution is limited to time-related differential equations, as illustrated in the figure.

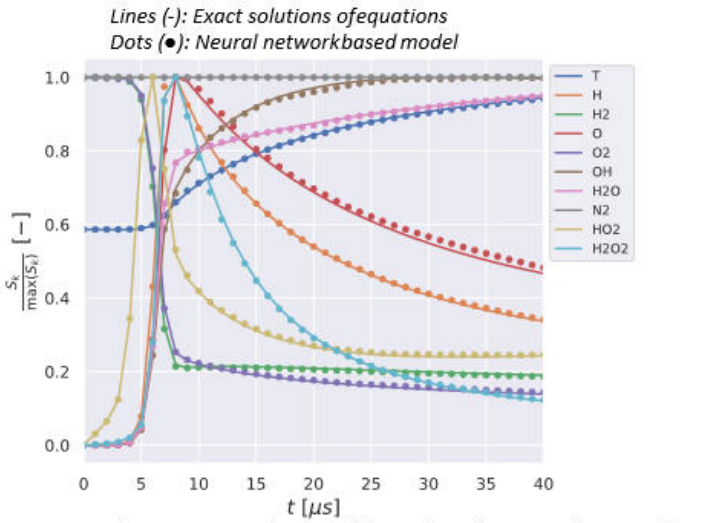
- Concerning the evolutions over time of the chemical species (figure), very good agreement was observed between the exact solutions and the solutions obtained with neural networks [1]. Increased accuracy was also observed for recurrent networks.

- A method was devised to construct neural networks that guarantee the conservation of mass of chemical elements [2].

Conservation equations:

$$\frac{dY_k}{dt} = \dot{\omega}_k, \qquad k = 1, \dots, N_S$$

$$\frac{dC_p T}{dt} = -\sum_k \frac{h_k}{W_k} \dot{\omega}_k$$



Comparison between Neural network based resolution and exact solution for hydrogen (H_2)

Neural network model:

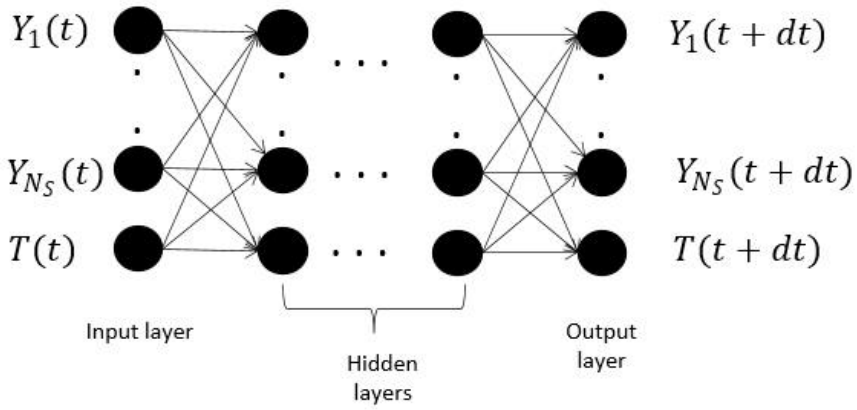


Illustration of the neural network resolution approach for the combustion of H2

This research illustrates the capacity of neural networks to replace chemical kinetics resolution algorithms. Future work on the method will focus on the following aspects:

- Deployment for cases of practical interest, through the definition of adapted learning databases.
- Evaluation of the calculation time savings compared to traditional methods.

Publications:

[1] *M. Guirat, T. Faney, C. Mehl,* ***Modeling of chemical evolution equations using Long Short Term Memory Neural Networks****, publication submitted.*

[2] *C. Mehl, T. Faney, patent under examination.*

Scientific contact: cedric.mehl@ifpen.fr

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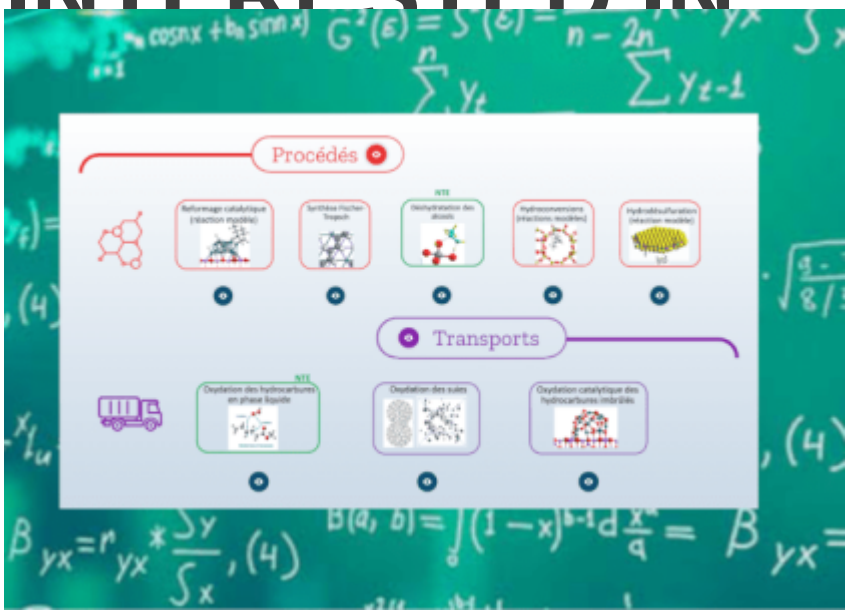


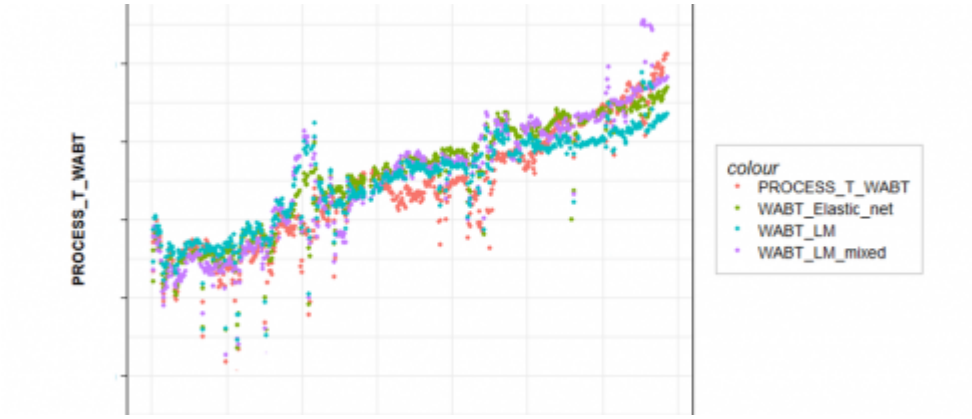
Fundamental Research

News

April 2021

Predicting performance from atomic through to reactor scales to improve industrial processes

Chemical sciences | Catalysis and reaction kinetics | Biosciences and biotechnologies | Biocatalysis



Mix between kinetic and machine learning models

Having access to increasingly precise and robust extrapolation models to be able to predict certain properties[a] remains a major challenge for chemical processes industry.

Engineering sciences | **Fluid mechanics** | **Chemical engineering and process engineering**
Systems modeling and simulation | **Mathematics and IT** | **Numerical methods and optimization**

Acceleration of chemical kinetics calculations through Machine Learning methods

A large number of simulators, whether they relate to the design of reaction processes, the evolution of oil reservoirs or combustion systems, require access to thermodynamic properties. In order to provide these properties, IFPEN has been developing a library of calculation modules, called “Carnot”, named after the famous French thermodynamics expert. These calculations, in particular those concerning phase equilibrium (also known as flash calculations), generally require the use of substantial calculation resources due to the complexity of the systems considered, and represent in many cases the most time-consuming step in the simulation process.

To address this, a PhD research project[1] set about developing a data-driven learning algorithm, leveraging neural networks, with a view to substituting it for existing flash calculations [1]. Three specific neural networks were established (figure 1) to:

- predict the number and type of coexisting equilibrium phases;
- initialize the distribution coefficients[2],K_i;
- evaluate the fugacity coefficients[3], ?_i used to update K_i.

Click on the picture to enlarge

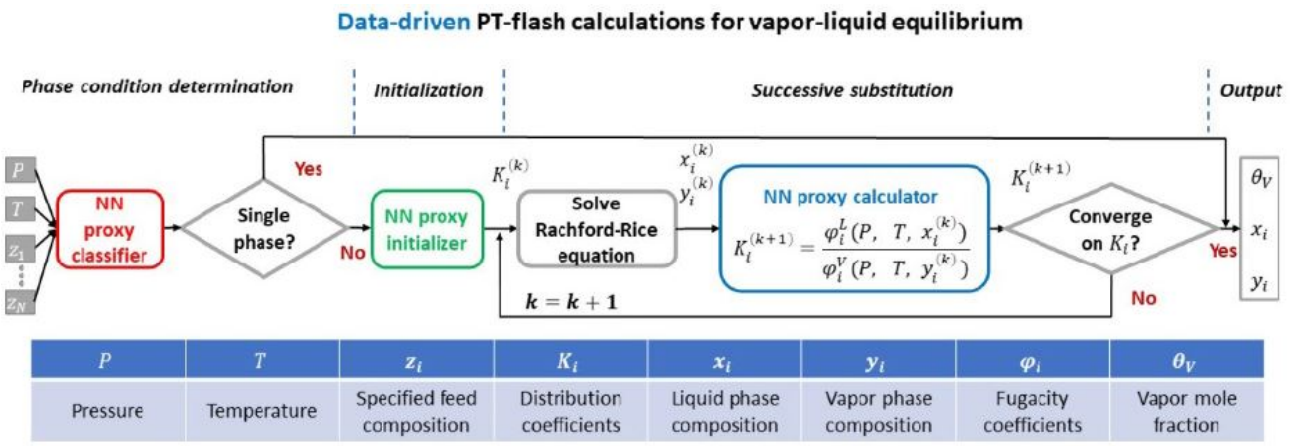


Figure 1: Chart of data-driven flash calculations

The need to scale up equilibrium calculations highlights the benefits of data-driven flash computations since one of the most compelling advantages of neural networks is that they lend themselves to parallel computation.

Our methodology was validated for a panel of experiments which delivered a 30-fold speedup in computation time (figure 2), **while maintaining a high degree of accuracy.**

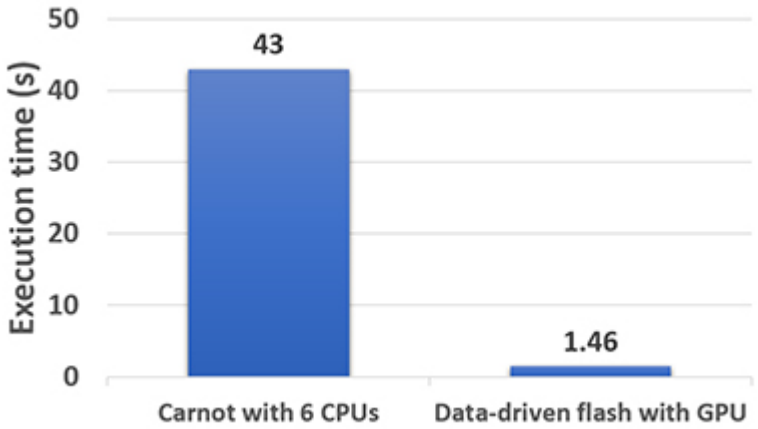


Figure 2: Comparison between the Carnot tool and data-driven flash in terms of execution time for 230,000 samples of a water/methane mixture.

The next steps will target the automation of the learning framework, for any given composition, and the integration into Carnot of the resulting statistical models, in order to evaluate the performance on simulations based on reference compositions.

In the longer term, the objective will be to optimize the learning process in real-time under the operating conditions specific to each numerical simulation scenario.

1- Jingang QU: “Acceleration of numerical simulations by means of deep learning - Application to thermodynamic equilibrium calculations”, ongoing IFPEN thesis
2- The distribution coefficient of the i-th component K_i corresponds to the ratio of the molar fraction of the i-th component between the gas and liquid phase.
3- The fugacity coefficient of the i-th component ?_i is the ratio between the real fugacity and the fugacity of the perfect gas in a mixture with the same pressure, temperature and composition.

Publication:

[1] *J. Qu, M. D’Heilly, P. Gallinari, J-C. de Hemptinne, T. Faney et S. Youssef,* ***Efficient phase equilibrium computations using learning algorithms****, ESAT 2021-31st European Symposium on Applied Thermodynamics, July 2021.*

Scientific contact: thibault.faney@ifpen.fr

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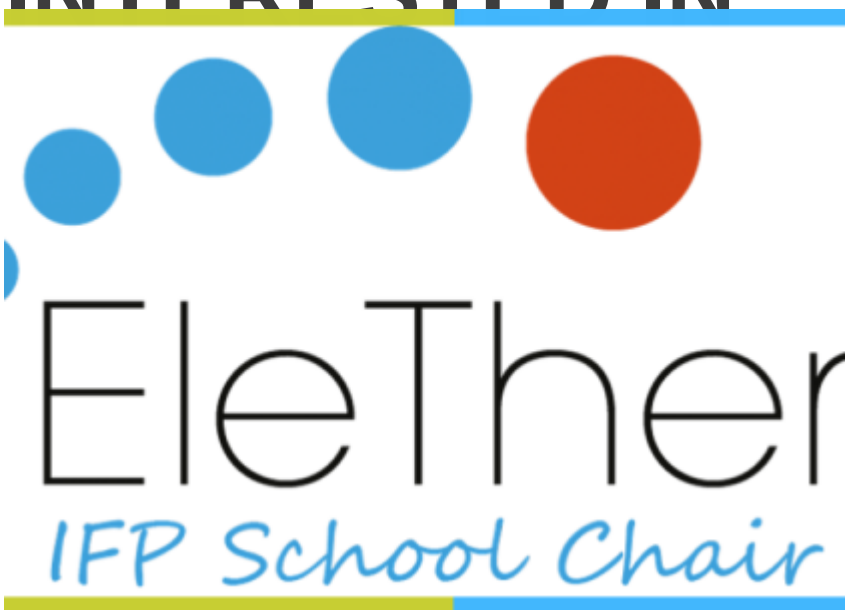
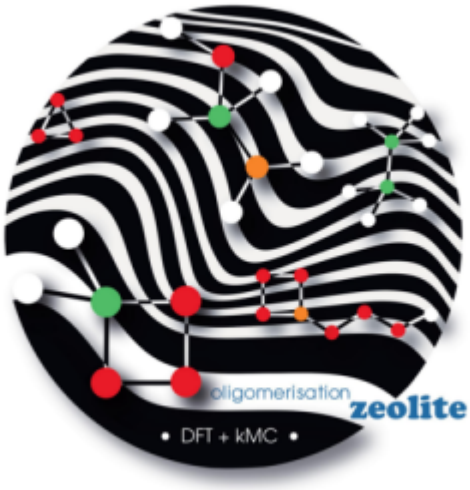


Training and Careers

News April 2021

New Chair on Electrolyte Thermodynamics

Physical Sciences | Thermodynamics/Molecular modeling



Fundamental Research

News March 2021

Molecular simulation methods contribute to the understanding of the early stages of zeolite synthesis

Chemical sciences | Catalysis and reaction kinetics | Physical Sciences | Thermodynamics/Molecular modeling

Faster “flash” calculations thanks to deep learning

The design of high-quality porous materials is a major challenge for the energy efficiency of industrial processes in the fields of catalysis and biocatalysis and separation and purification operations. For such applications, these materials derive their properties of interest from their specific microstructure, incorporating a large quantity of empty spaces that are organized and connected on a nanometric scale. IFPEN and Saint Gobain Research Provence (SGRP) joined forces to acquire a tool that will ultimately facilitate the development of porous materials optimized for given usages[1]. The partners adopted an innovative approach based on digital twins, developed from random microstructure models and adjusted using numerical models that imitate experimental procedures. This approach was then validated by comparison with test results on model microstructures.

Numerical simulation of experimental aspects is conducted on simulated three-dimensional microstructures [1] and is based on a geometric approach. Hence the approach adopted primarily uses correlations between the morphological parameters and physical quantities that characterize the system under consideration. It is this transition from a description of quasi-static states of physicochemical mechanisms - such as phase equilibrium changes - to the purely geometric and morphological description of the phenomena at play that represents the biggest difficulty to be overcome.

Mathematical morphology, a scientific field that has long focused on the characterization of the 2D and 3D textural properties of microstructures, proved invaluable to the resolution of this challenge. To construct the digital material, specific pore network extraction algorithms [2] firstly made it possible to consider pores with complex and random geometries, similar to those encountered in real materials (figure). Mathematical morphology operators[2] were then used to simulate the phenomena involved in experimental porosimetry techniques. In particular, an operator of interest for these porous networks was estimated: tortuosity (figure), a property closely related to diffusion phenomena since it characterizes ease of flow across these networks [3].

With this type of digital twin approach, experimental simulations can take into account large representative volumes, with multi-scale and multi-structure arrangements, with reasonable calculation times.

In order to further optimize calculation time without compromising the precision of results, deep learning is a promising tool currently being evaluated to establish a direct link between digitized microstructures and simulated test results.

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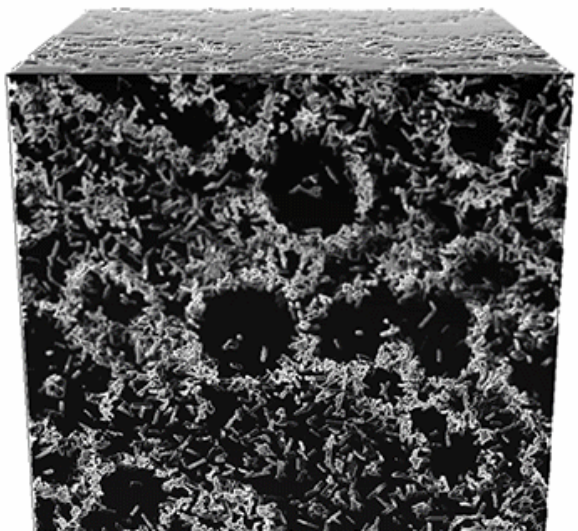

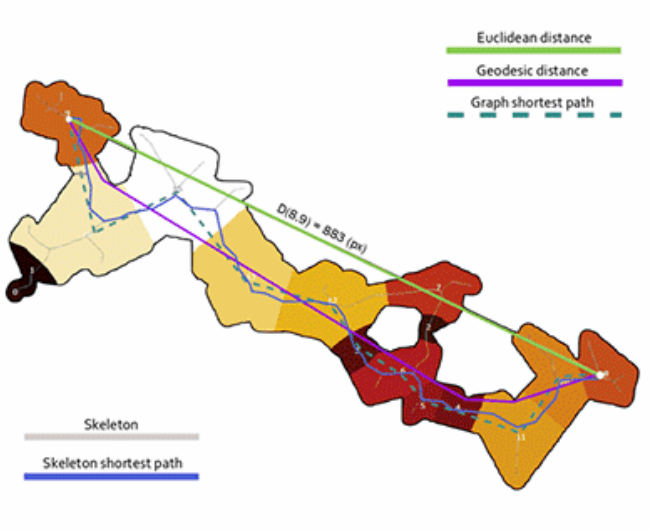

On the left, numerical simulation of the microstructure of a porous material.
On the right, illustration of a tortuosity operator, ratio of the lengths of paths between two points “as the crow flies” (Euclidean distance) and constrained by the porous network (geodesic distance).

1- This research, launched in 2019, has been the focus of post-doctoral work conducted by Alexey Novikov and the PhD thesis research currently being conducted by Adam Hammoumi.
2-See examples at https://fr.wikipedia.org/wiki/Morphologie_math%C3%A9matique

---

Publications:

[1] *M. Moreaud, J. Chaniot, T. Fournel, J.M. Becker, L. Sorbier.* ***Multi-scale stochastic morphological models for 3D complex microstructures****. 17th Workshop on Information Optics (WIO), IEEE Conference (2018).*
>> https://doi.org/10.1109/WIO.2018.8643455

[2] *A. Hammoumi, M. Moreaud, E. Jolimaitre, T. Chevalier, A. Novikov, M. Klotz.* ***Efficient Pore Network Extraction Method Based on the Distance Transform. International Conference on Artificial Intelligence & Industrial Applications****. Springer Ed. (2020).*
>> https://doi.org/10.1007/978-3-030-53970-2_1

[3] *A. Hammoumi, M. Moreaud, E. Jolimaitre, T. Chevalier, A. Novikov, M. Klotz.* ***Graph-based M-tortuosity estimation****. IAPR International Conference on Discrete Geometry and Mathematical Morphology (2021).*

Scientific contact: Maxime Moreaud

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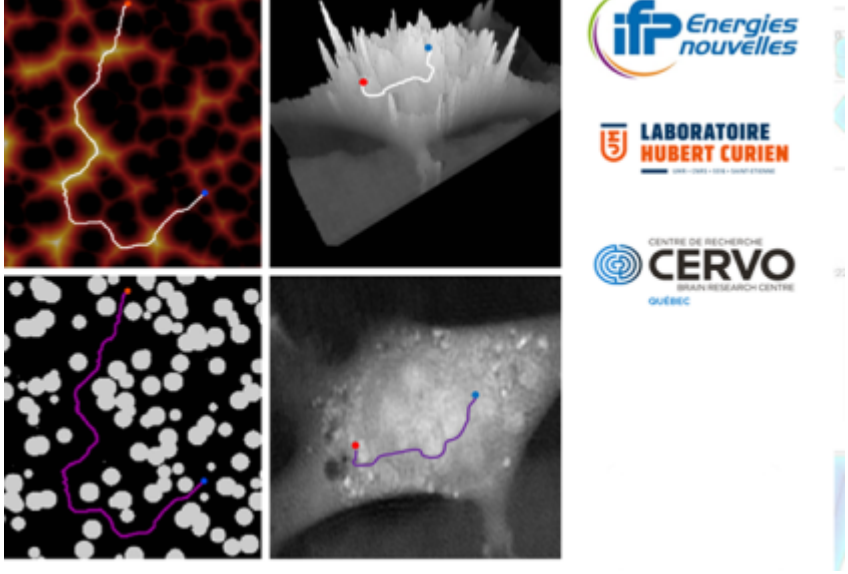


Fundamental Research

News December 2019

New porous microstructure descriptors based on tortuosity and accessibility

Geosciences | Petrophysics and transfers in porous media | Analysis and characterization | Structural analysis and Imaging | Mathematics and IT | Signal processing/Data science

Numerical design based on the analysis of multi-scale porous material microstructures

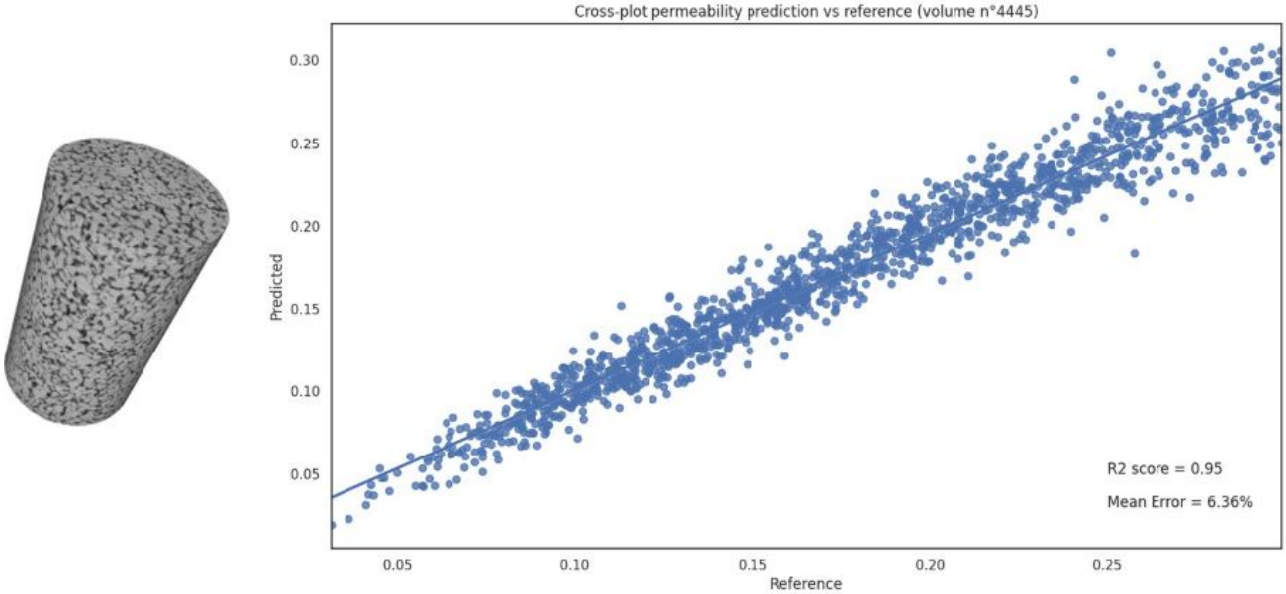
Today, characterization of geological reservoirs, a long-standing theme in petroleum exploration, becomes a base of interest for a variety of applications, such as CO_2 and hydrogen storage as well as geothermal energy. In recent years, the combined use of 3D microtomography (or micro-CT[1]) imaging and advanced simulation techniques has allowed the emergence of a digital approach to computing the petrophysical properties of reservoir rocks (Digital Rock Physics). This represents a real complement - and in some cases an alternative - to traditional laboratory measurements.

To this end, IFPEN has carried out an unprecedented tomographic image acquisition campaign, using the PSICHE beamline of the SOLEIL synchrotron, on a hundred rock samples (1 cm in diameter and 2 cm in length). The voluminous and exclusive database[2] of 3D images thus generated was then used to predict petrophysical properties.

Usually, numerical methods used to compute physical properties from 3D images[3] are very time-consuming and often limited by the resolution of these images. For this work, researchers at IFPEN have deployed an alternative method based on Deep Learning, capable of fully exploiting the large volume of acquired data [1]. This ambitious approach allowed to reconcile the huge amount of data with neural architectures, drawing on 3D convolutional neural networks[4]. It required the use of large parallel calculation resources, such as graphic processors[5], accessible on the Jean-Zay supercomputer of GENCI[6].

These calculations led to a good prediction performance concerning the permeability of the studied rocks (figure)**, thereby demonstrating the potential of deep learning methods in the field.**

Click on the picture to enlarge



Example of 3D digital sample and comparison of permeability prediction on the y-axis versus the experimental reference on the x-axis

However, questions remain concerning the generalization of the prediction quality to other rocks and research is underway to confirm its relevance for this use.

A first aspect of this research consists in using learning methods further upstream, for example to deduce properties of interest, at the voxel scale. **The ambition is to predict velocity fields at all points of the volume to enable more accurate permeability calculations.**

The other aspect concerns the use of specific neural architectures to improve the resolution of the images acquired, a major challenge for the implementation of learning models.

1- Micro Computed Tomography
2- 32 Go memory for each plug due to digitalization with a resolution of 5.8 µm
3- Such as Porous Network Modeling (PNM) or the Lattice Boltzmann Method (LBM)
4- Multilayer neural networks with a connection architecture inspired by that of the visual cortex of mammals
5- Graphic Processor Unit (GPU)
6- National High-Performance Computing Equipment

Publication:

[1] *S. Youssef, G. Batot, F. Cokelaer, S. Desroziers et M. Feraille*, ***On the Performance of Deep Learning Methods for Rock Property Prediction from 3D Micro-CT Images***, *currently being drafted*

Scientific contact: souhail.youssef@ifpen.fr

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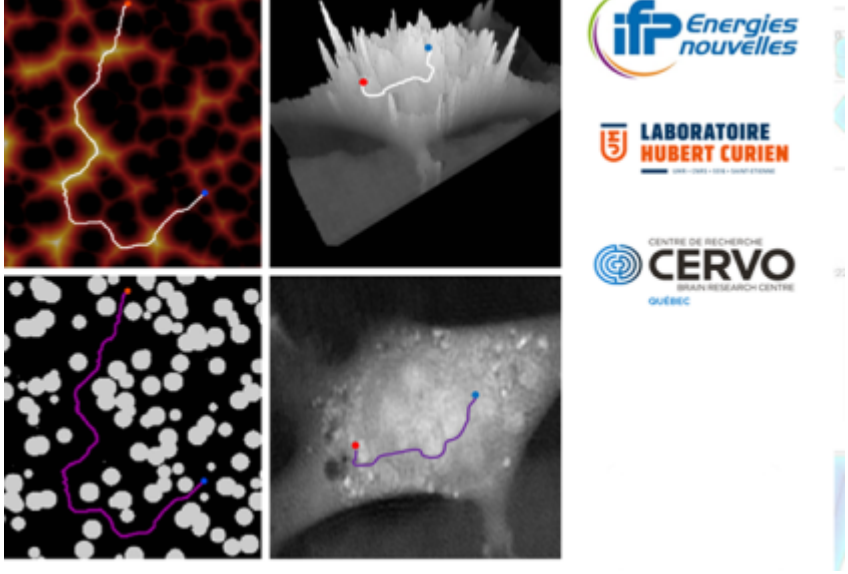

Fundamental Research

News December 2019

New porous microstructure descriptors based on tortuosity and accessibility

Geosciences | Petrophysics and transfers in porous media | Analysis and characterization | Structural analysis and Imaging | Mathematics and IT | Signal processing/Data science

Digital Rock Physics at IFPEN

Over the last decade, deep learning applied to image analysis has rapidly developed in scope to cover numerous fields. However, its potential remains underexploited in geology, despite the fact that it is a discipline that relies to a large extent on visual interpretation. To contribute to the digital transformation of industries related to the underground environment, researchers at IFPEN have implemented deep learning in three "profession-specific contexts", each involving different types of geological images.

The first application [1] is an image classification of macroscopic rock samples with convolutional neural networks[1].

Researcher began by implementing and comparing different neural architectures and learning strategies considered in the scientific literature as references for image analysis. This enabled them to construct a first effective prediction tool.

They then adopted an original approach mirroring that of a geologist, based on a cascade-neural-network model tree. This method facilitates the integration of geological knowledge in the statistic model and offers an increased capacity to explain predictions. It also complements the first model by compensating for certain errors (Figure 1).

Click on the picture to enlarge

Figure 1: Automated classification of field samples with artificial intelligence algorithms.
Top: direct classification. The three most likely classes according to the neural network are displayed on each image. The first two images are archetypal and probabilities clearly point to a single class. However, the third image is more ambiguous and the probabilities reflect the uncertainties a human geologist would be faced with.
Bottom: lithological classification combining recognition of the petrological characteristics and a decision tree.

In the second application [2], detection algorithms were employed to define and categorize microfossils on digitized images of thin rock sections.

Several deep learning methods for the detection of objects, based on the state of the art, were compared for a first set of data limited to 15 annotated images. The results for 130 other images of thin sections were qualitatively evaluated by expert sedimentologists, with quantitative measurements of precisions and inference times[2]. This work constitutes a proof of concept for the automated identification of paleofauna, since models demonstrated a good capacity to detect and categorize microfossils (Figure 2). However, differences in precision and performance were highlighted, leading to recommendations being made for their use in similar projects.

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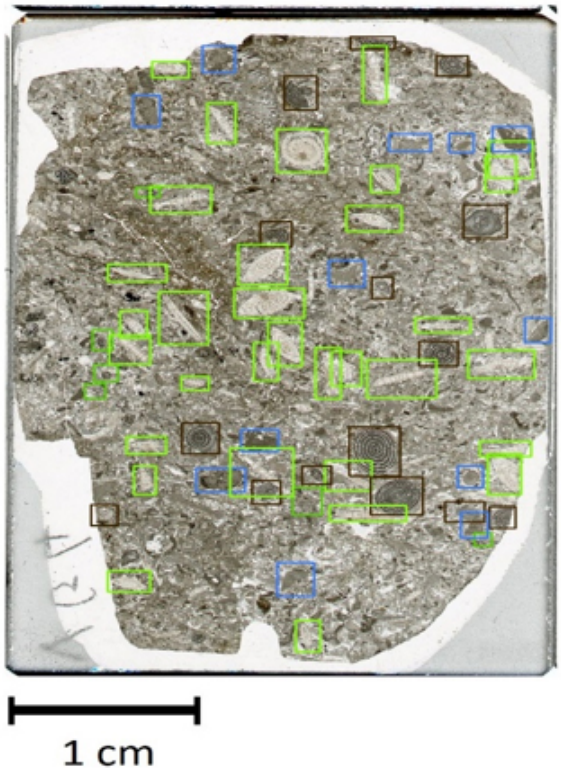

Figure 2: Automated microfossil detection on a thin rock section. Each rectangle generated by the algorithm defines a zone containing a microfossil. Its color corresponds to the most likely species according to the model (e.g., green for nummulites, brown for alveolinids)

The third application [3] is an automated lithological characterization of geological core images. The data considered come from an IODP (International Ocean Drilling Program) drilling campaign in the

Corinthian Gulf. They were gathered at 3 different sites and were interpreted by an expert in 17 facies associations. In this work, different challenges and potential solutions were highlighted in order to manage situations in which little training data is available. In particular, transfer learning[3], as well as hyperparameter calibration[4], prove to be crucial for the development of an effective predictive system.

This body of research highlights the potential of deep learning methods to obtain relevant geological information from images, while underlining the importance of adapting them to the specific applications concerned.

1- Multilayer neural networks with a connection architecture inspired by that of the visual cortex of mammals.
2- Deduction process based on implicit information
3- Consisting of applying knowledge obtained by carrying out a task in order to solve a different problem but with certain similarities.
4- In machine learning, a hyperparameter is a variable the value of which is used to control the training process.

Publications:

[1] *A. Bouziat, S. Desroziers, M. Feraille, J. Lecomte, R. Divies et F. Cokelaer,* ***Deep Learning Applications to Unstructured Geological Data: From Rock Images Characterization to Scientific Literature Mining****, First EAGE Digitalization Conference and Exhibition, Nov 2020, Volume 2020*
>> https://doi.org/10.3997/2214-4609.202032047

[2] *A. Koroko, A. Lechevallier, M. Feraille, J. Lecomte, A. Bouziat et S. Desroziers,* ***Appraisal of several Deep Learning models for microfossil identification on thin section images****, Second EAGE Workshop on Machine Learning, Mar 2021, Volume 202,*
>> https://doi.org/10.3997/2214-4609.202132005

[3] *A. Lechevallier, A. Bouziat et S. Desroziers,* ***Assisted interpretation of core images with Deep Learning workflows: lessons learnt from a practical use case****, Second EAGE Workshop on Machine Learning, Mar 2021, Volume 2021,*
>> https://doi.org/10.3997/2214-4609.202132003

Scientific contacts: antoine.bouziat@ifpen.fr and sylvain.desroziers@ifpen.fr

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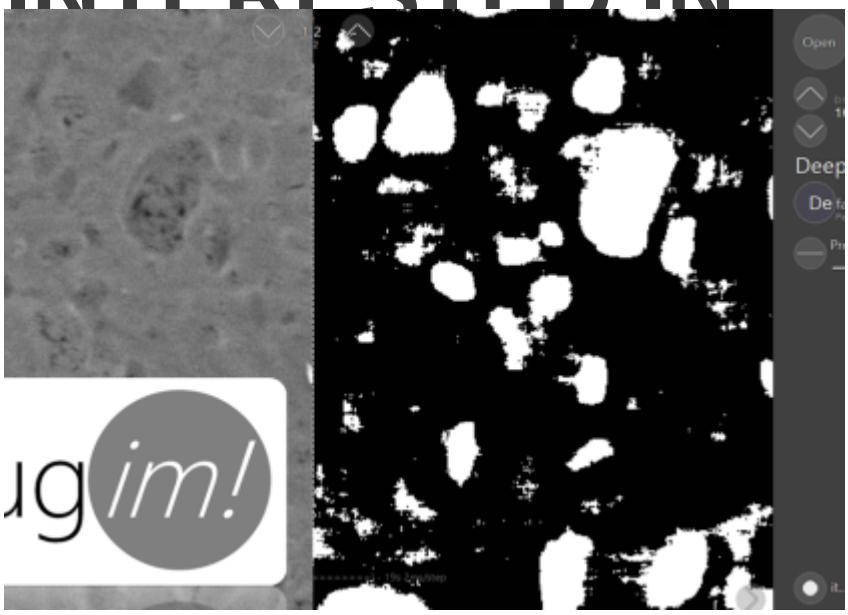

Fundamental Research

News June 2019

Integration of deep learning in IFPEN projects

Mathematics and IT | Signal processing/Data science | Software design

Artificial Intelligence-assisted interpretation of geological images

Image analysis is widely used for the microstructural characterization of materials. Digital microscopy images provide representative magnitudes of the texture, which impact global properties (for example diffusion or mechanical).

Semantic segmentation conducted on microscopy images is a processing operation carried out to quantify a material's porosity and its heterogeneity. It is aimed at classifying every pixel within the image (on the basis of degree of heterogeneity and porosity). However, for some materials (such as aluminas employed for catalysis), it is very difficult or even impossible using a traditional image processing approach, since porosity differences are characterized by small contrasts and complex textural variations.

One way of overcoming this obstacle is to tackle semantic segmentation via deep learning, using a convolutional neural network[1]. This method, here supervised, requires a reference base built on microstructural images and their hand-segmented equivalents in which the pixels in each zone have been assigned a binary value (0 or 1) corresponding to their degree of porosity (high / low). The creation of this base is extremely laborious and can only be considered for a limited number of images.

During the learning phase, the network learns to convert a gray scale image (8 bit code[2]) into its binary equivalent, thereby differentiating the forms of heterogeneities present in the microstructure. Learning takes place on reduced zones (patches), both to increase the number of data (several patches per image) and to facilitate learning with a smaller network, comprising fewer parameters to be optimized [1]. This particular way of proceeding, made necessary by the limited size of the learning base, may lead to imprecisions on the edges of the subsections. A sampling strategy stochastically assembling the patches predicted by the network is then used to compensate for this effect (figure).

These new image analysis opportunities based on deep learning, combined with traditional techniques, provide fresh and unprecedented data that can be used to guide the manufacture of porous materials. This segmentation method has been successfully used to characterize different types of alumina catalyst supports [2], after a peptization operation aimed at providing the porous network with a hierarchical organizational structure[3].

In the different zones of textural heterogeneity observable using scanning electron microscopy, porosity was quantified using a new measurement method on a local scale [3]. Combined with the hypothesis of a dense barrier formed around the zones of highest porosity, these new results explain the effective differences in diffusion properties macroscopically measured on catalyst supports [2].

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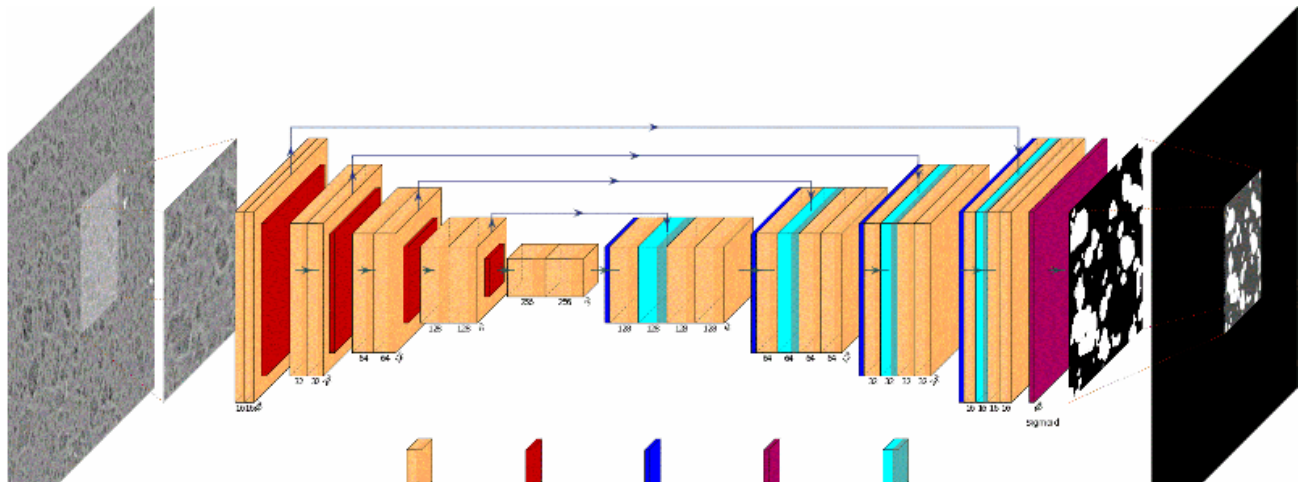

Illustration describing the semantic segmentation of a microscopic image into different zones of porosity heterogeneity with a convolutional neural network. The output image is reconstituted from random patches extracted from the input image.

1- Multilayer neural networks with a connection architecture inspired by that of the visual cortex of mammals
2- Value of each pixel between 0 and 255
3- With dimensions ranging from the nanometric to the millimetric scale

---

Publications:

[1] *A. Hammoumi, M. Moreaud, C. Ducottet, S. Desroziers,* ***Adding geodesic information and stochastic patch-wise image prediction for small dataset learning****, Neurocomputing, 2021, ISSN 0925-2312*
>> https://doi.org/10.1016/j.neucom.2021.01.108

[2] *A. Glowska, E. Jolimaître, L. Catita, M. Fleury, T. Chevalier, S. Humbert, A. Hammoumi, M. Moreaud, L. Sorbier, MO. Coppens,* ***Multi-technique characterization of hierarchically organized gamma-alumina catalyst supports****, Under preparation, 2021.*

[3] *L. Sorbier, H. Poncet, V. Lecocq, G. Maillet, M. Moula, V. Le Corre,* ***Local porosity measurement from scanning electron microscopy images in the backscattered electrons mode****, Microscopy and Microanalysis, 27(1), 20-27, 2021*
>> https://doi.org/10.1017/S1431927620024782

Scientific contacts: Maxime Moreaud and elsa.jolimaitre@ifpen.fr

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24 - 25 November 2020

MATERIAL SYNTHESIS (2020)

Chemical sciences | Organic and mineral synthesis | Engineering sciences | Chemical engineering and process engineering | Systems modeling and simulation

Semantic segmentation through deep learning in materials sciences

Issue 45 of Science@ifpen - Special issue Data Science
21 June 2021

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