INFERENCES - RESEAUX DE NEURONES
LOIS PHYSIQUES

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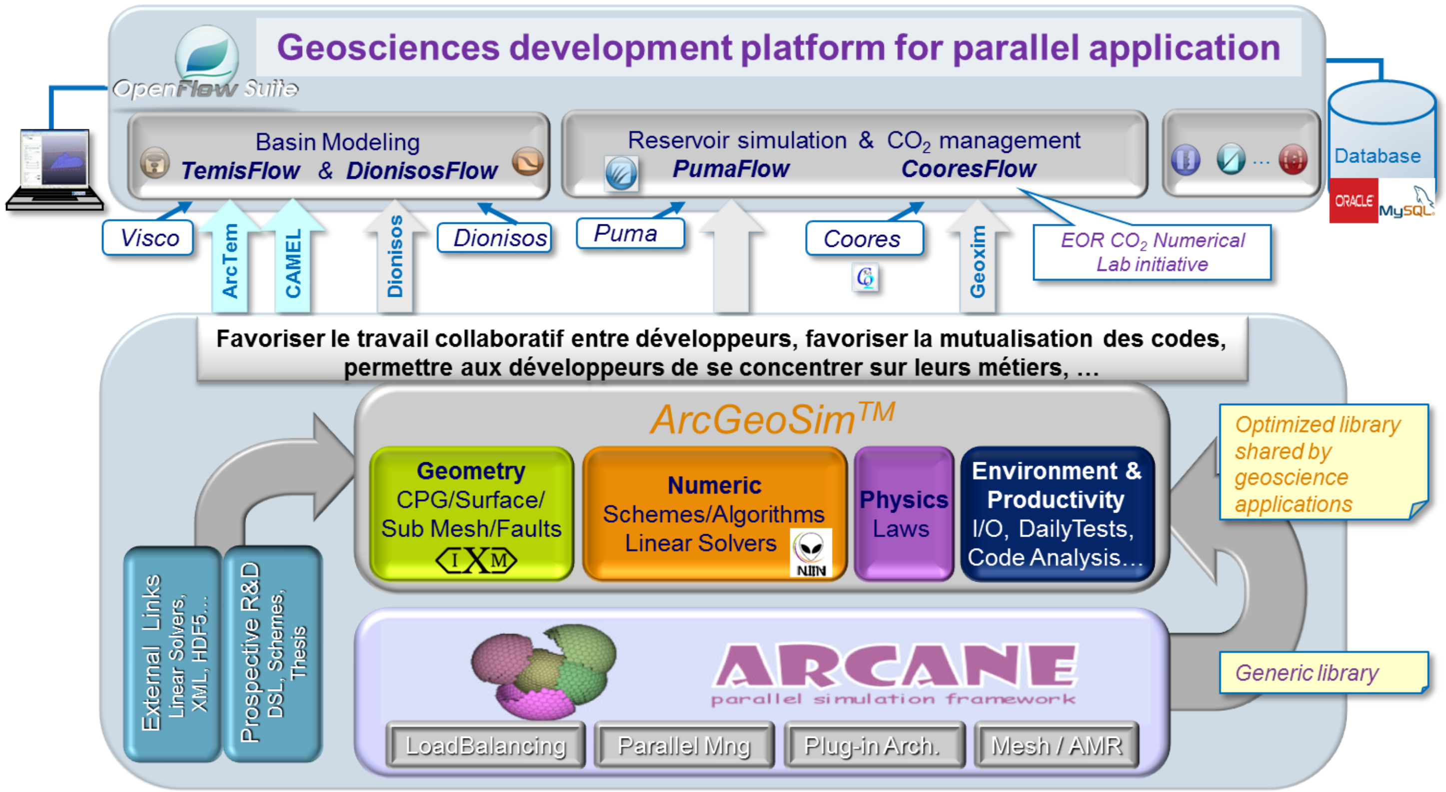
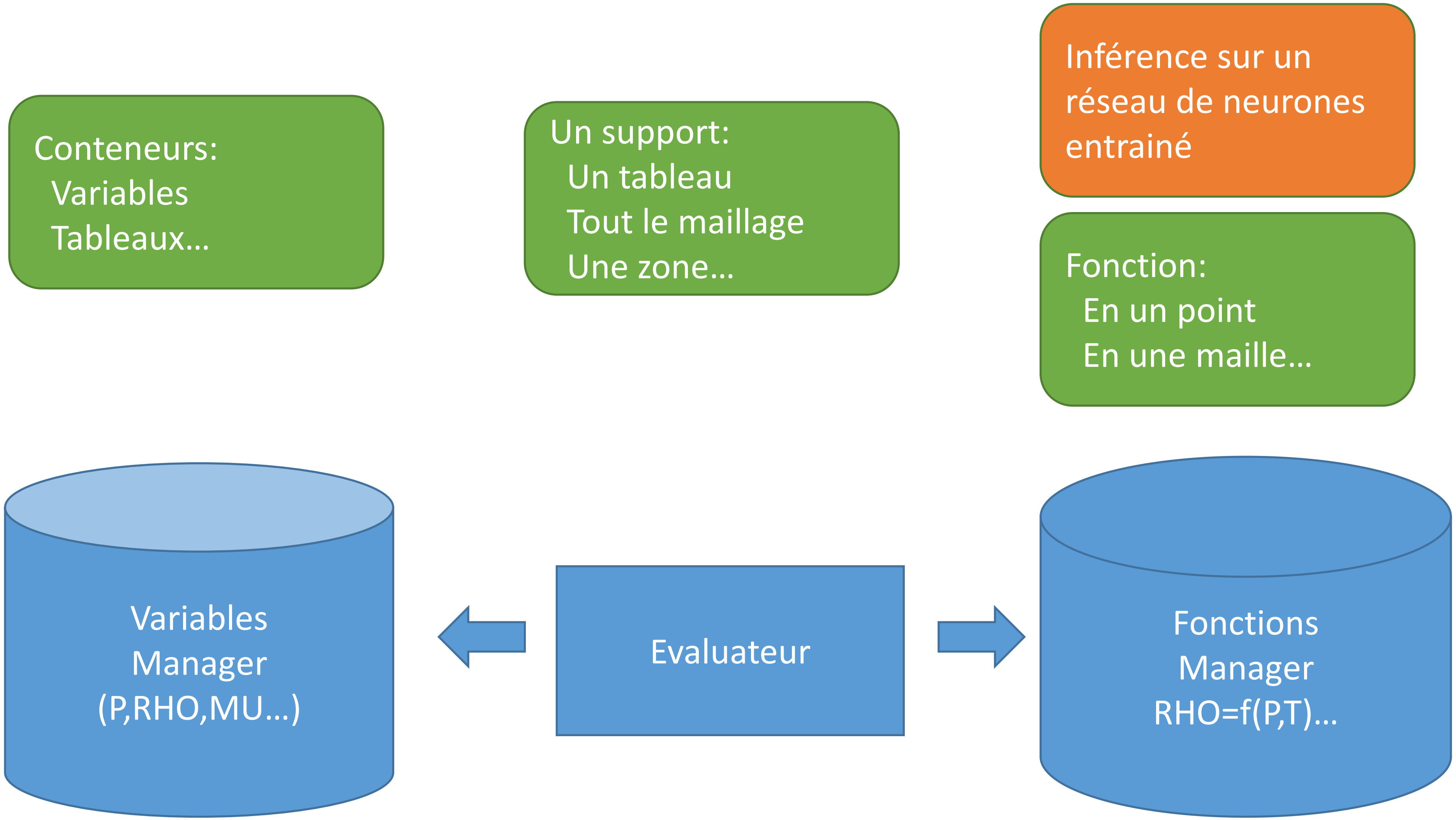
R. LEMORE - I. FAILLE
17-04-2023

LOIS - ARCGEOSIM - APPLICATIONS



LOIS PHYSIQUE API



SÉLECTION D’UN FRAMEWORK D’INFÉRENCE C++

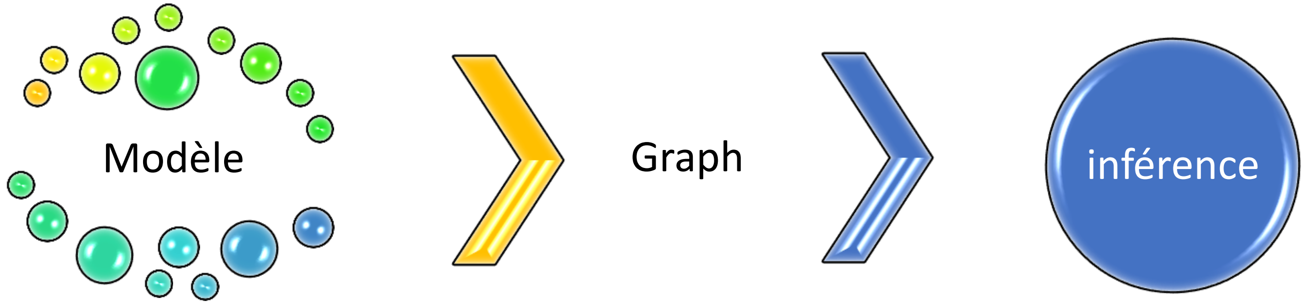
SÉRIALISATION ET INFERENCES

- Sérialiser :

  écrire le modèle d’une manière sérielle structurée sous forme de dictionnaire

- Inférer :

  désérialiser le modèle et de le remettre sous sa forme initiale de graph puis de faire des prédictions avec différentes entrées et obtenir les réponses



Création et entraînement en Python

PyTorch, TensorFlow

Formats

.pt, .pb, .onnx

Inférence C++

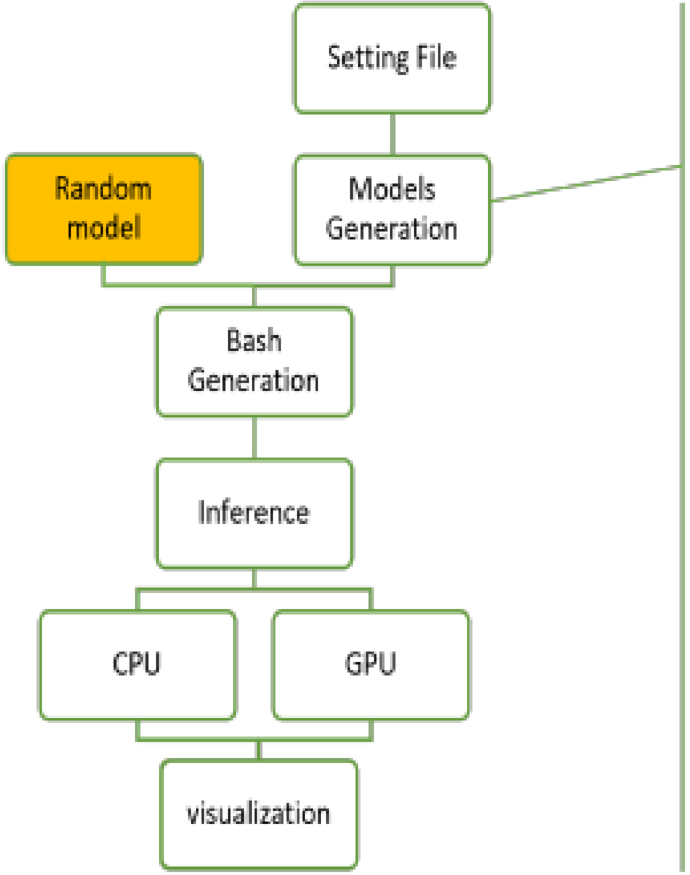
Torch,

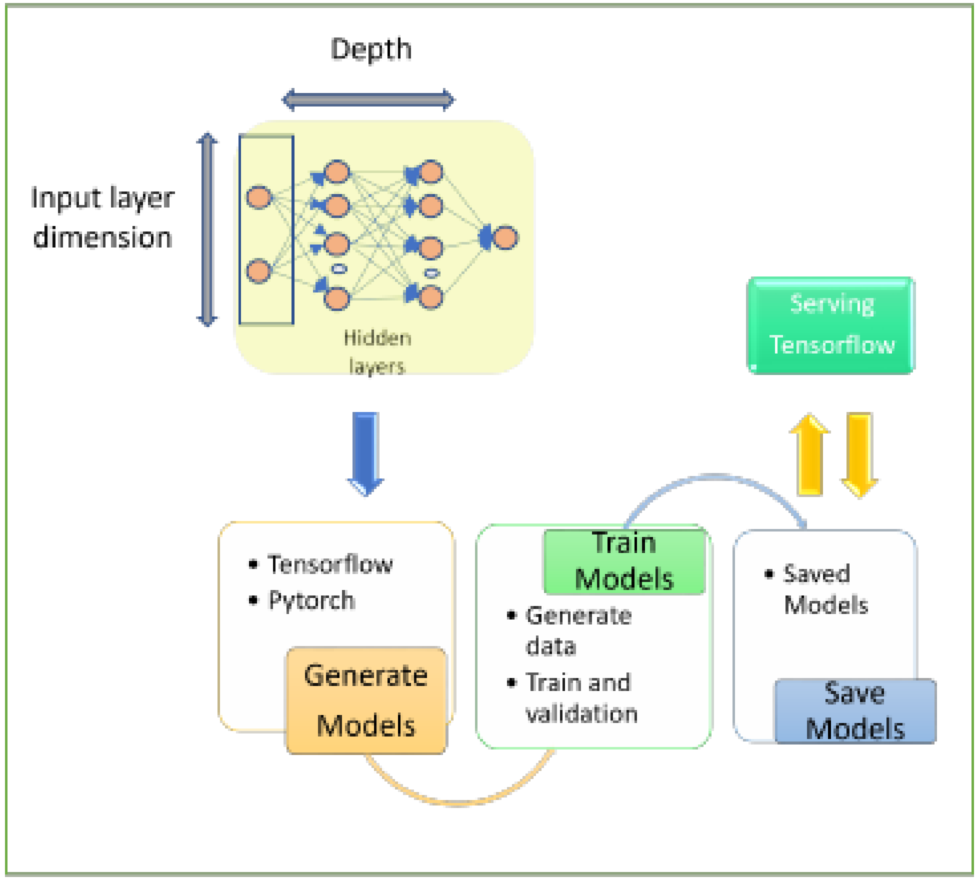
TensorFlow,

ONNXRuntime

PLATEFORME DE BENCHMARK

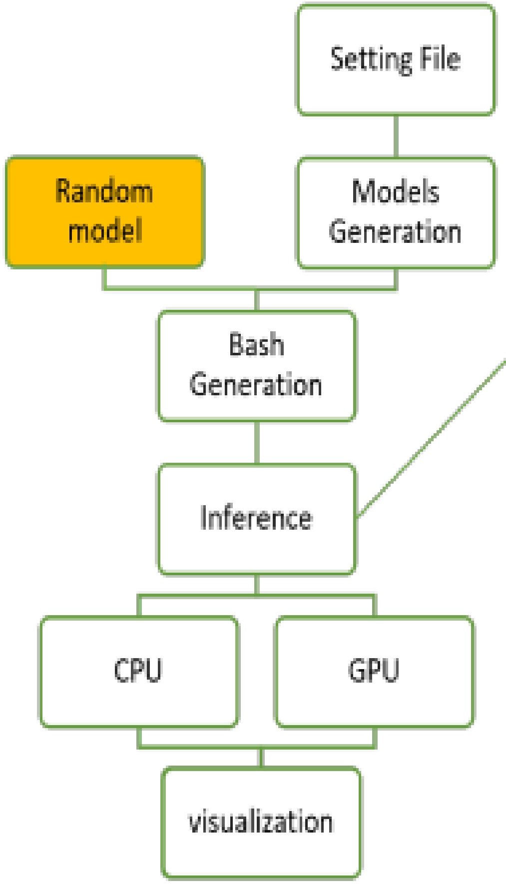
ENTRAINEMENT: PYTORCH, TENSORFLOW…

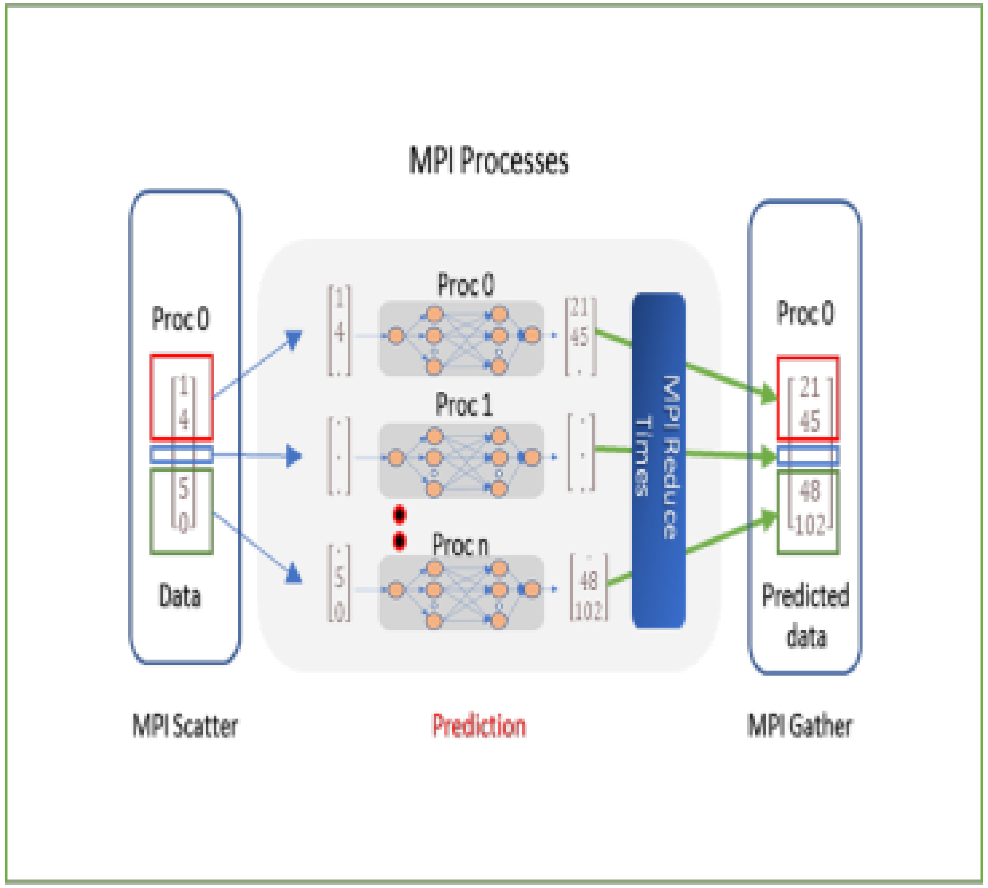




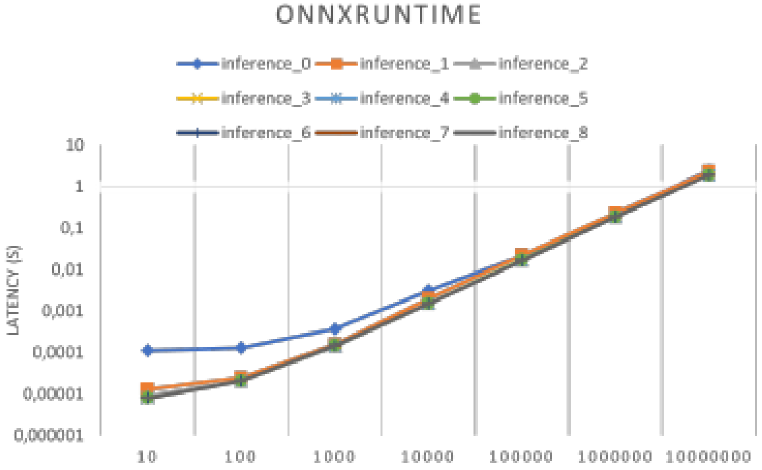
PLATEFORME DE BENCHMARK

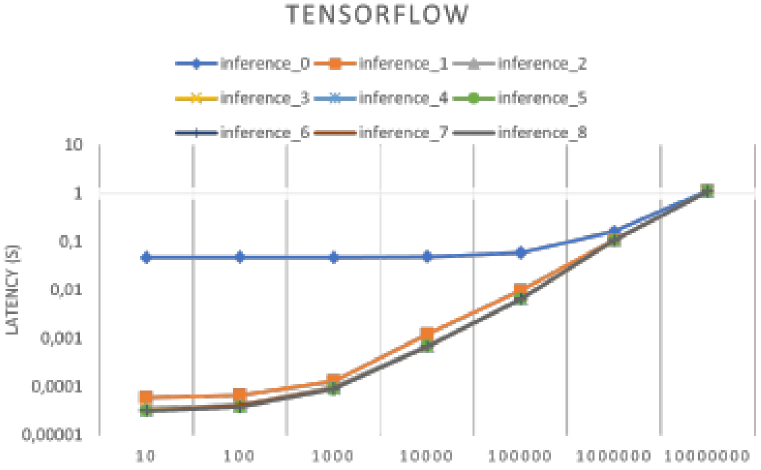
INFERENCE: TORCH, TENSORFLOW, ONNXRUNTIME…

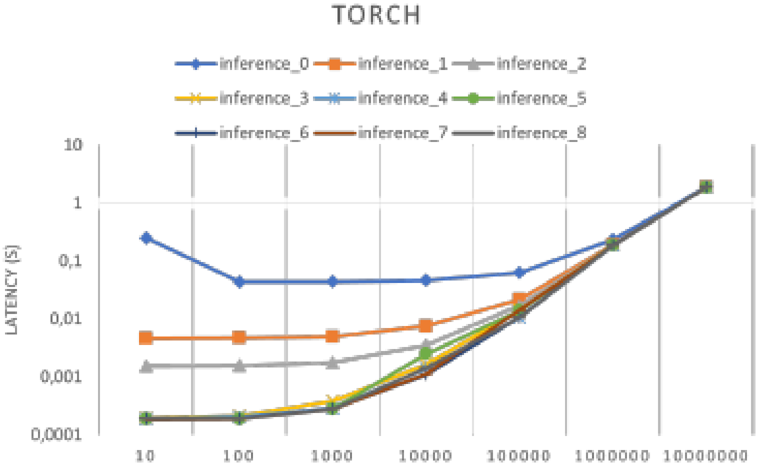




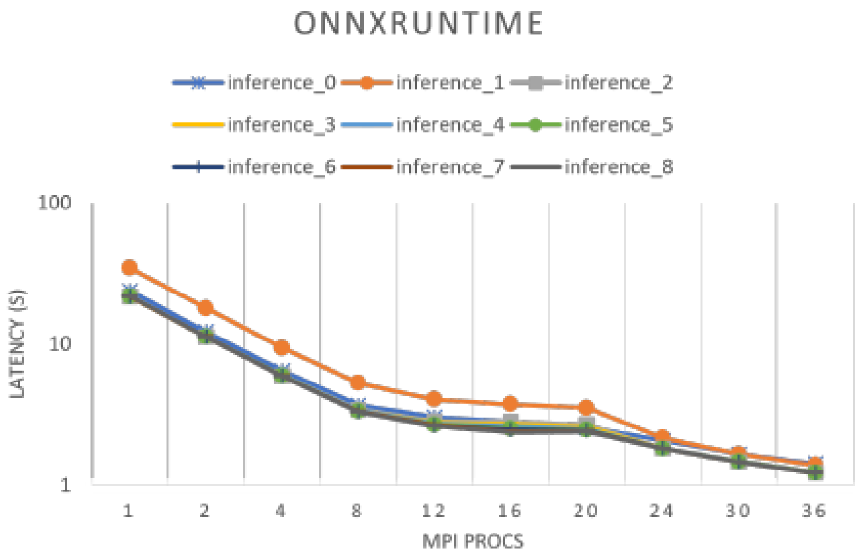
MODÈLE NON LINÉAIRE FONCTION DU BATCH SIZE (MONDELE:NL 1-4-16-32-1)

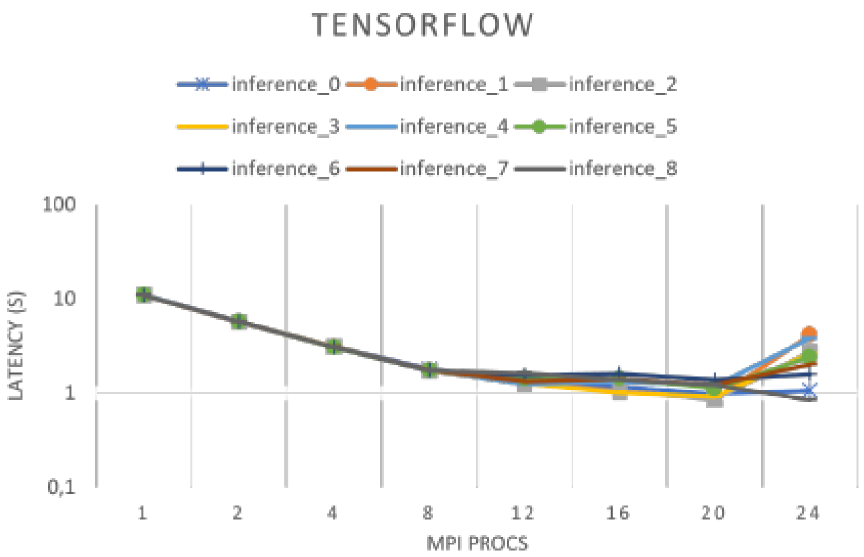


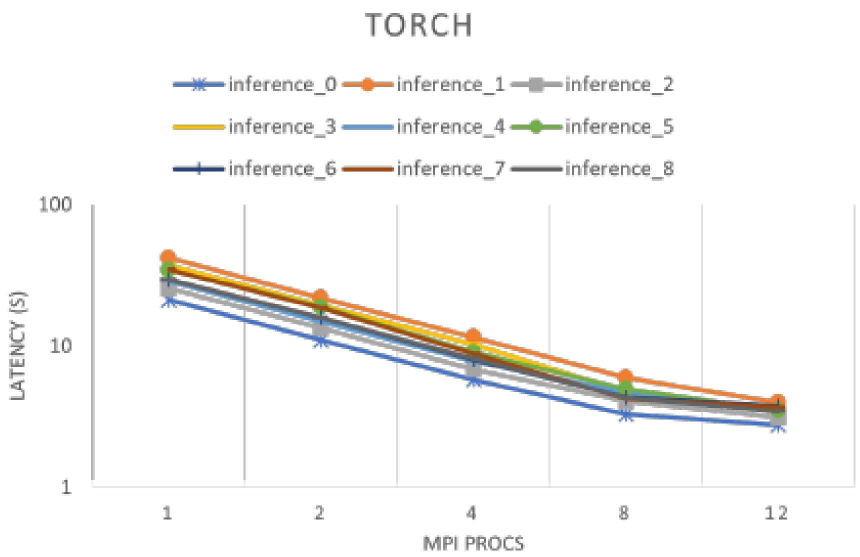




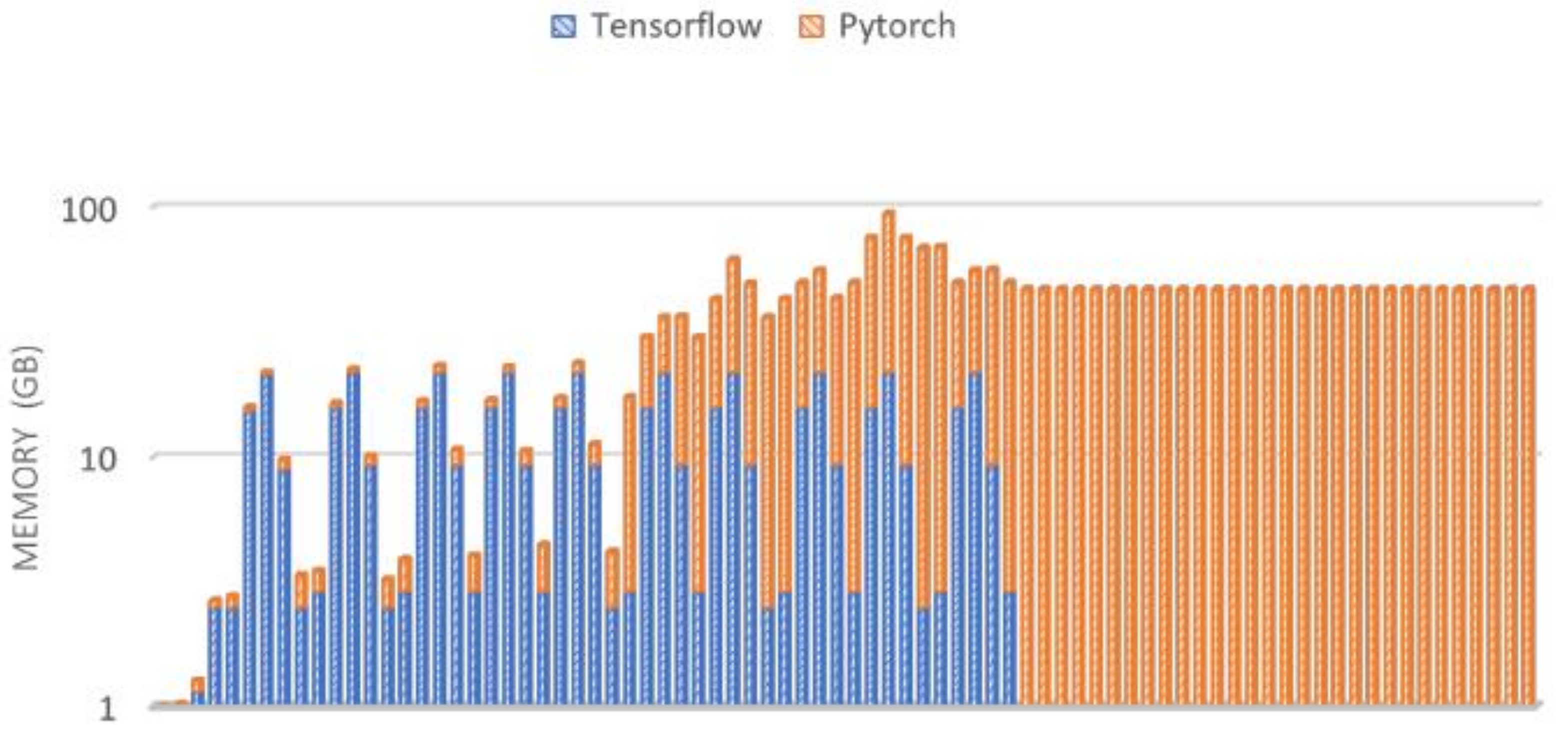
SCALABILITE MPI (MONDELE:NL 1-4-16-32-1, BATCH SIZE=10E8)



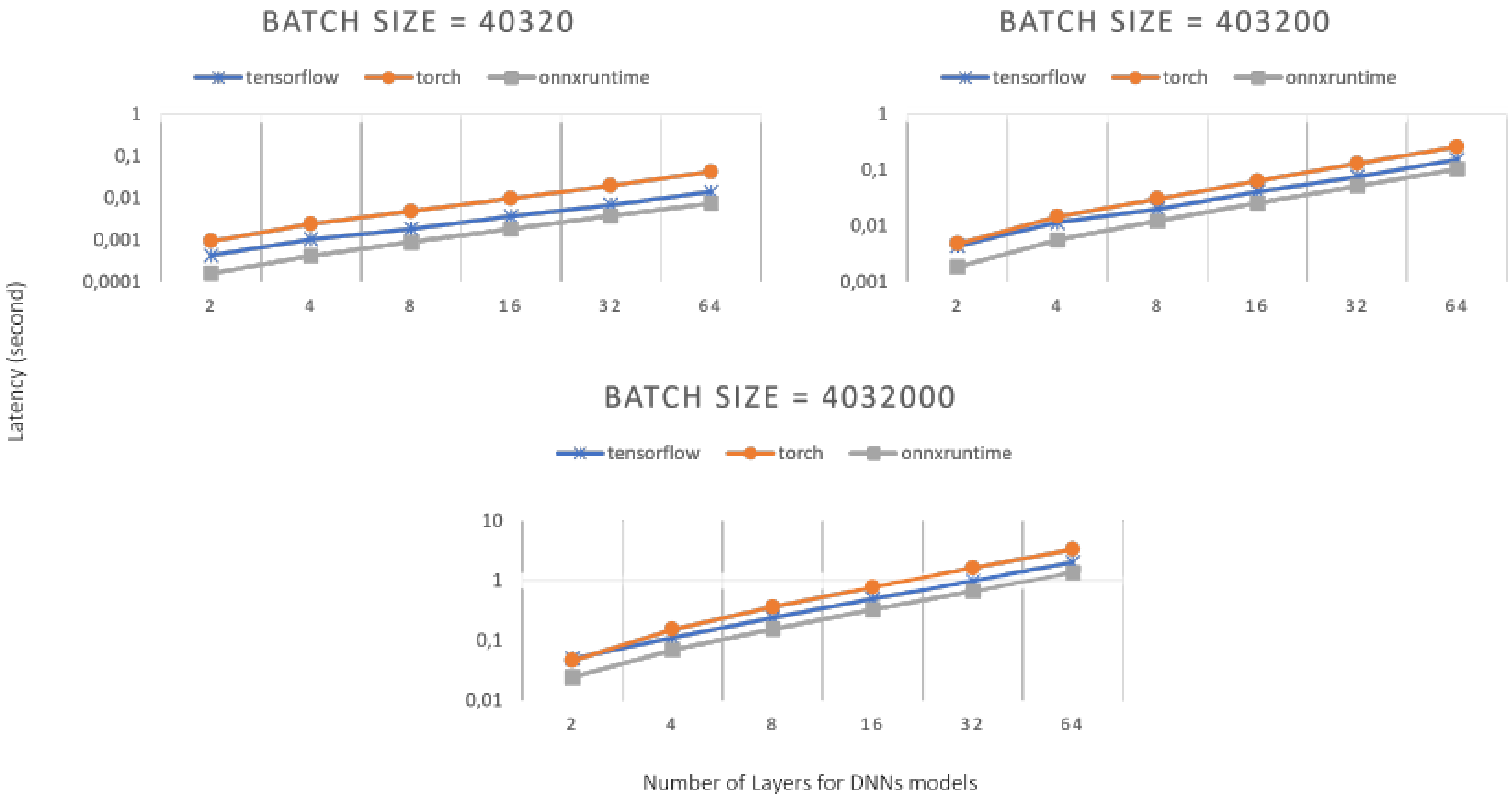




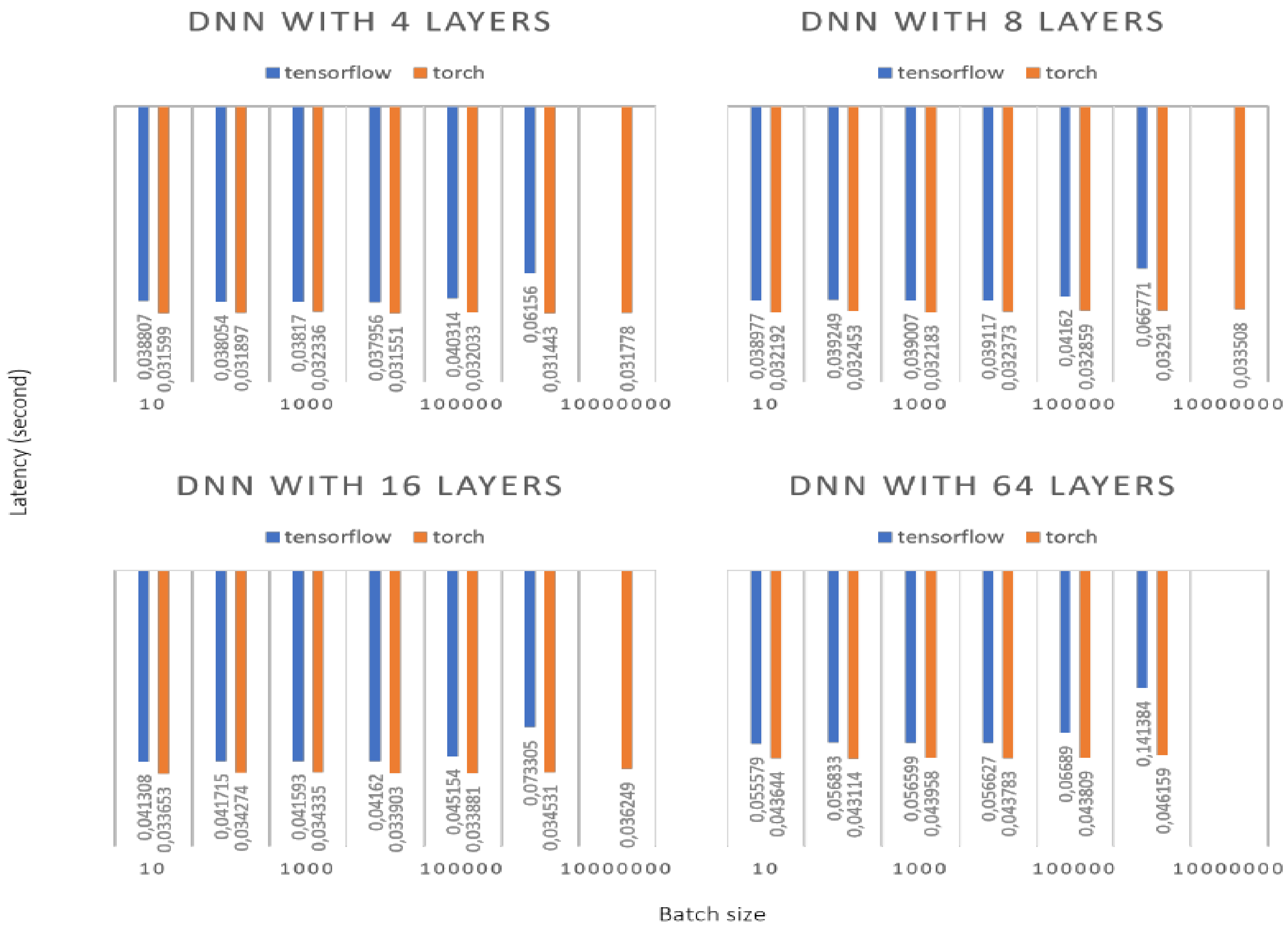
PROFILAGE MÉMOIRE



SCALABILITE NOMBRE DE COUCHE DU DNN (2-10N-2)



SCALABILITÉ SUR GPU



LOI DNN « GETUP » DANS GEOXIM

LAWS GEOXIM: SOLID PHASE ELASTIC PROPERTIES

- Elastic properties : computation in several stages
- Solid System bulk and shear moduli (K_s, G_s)
  - Standard averages
    - Voigt bound (arithmetic) : $M_v = \sum_{\alpha\ solid\ phase} F_\alpha M_\alpha$
    - Reuss bound (harmonic) : $\frac{1}{M_R} = \sum_{\alpha\ solid\ phase} F_\alpha \frac{1}{M_\alpha}$
    - Voigt-Reuss-Hill average $M_{VRH} = \frac{1}{2}(M_v + M_R)$
  - If no Reactive Transport
    - SolidElasticModuliLawConfig
    - Solid elastic properties are given in tables
  - With reactive Transport
    - GeochemicalSolidElasticModuliLawConfig
    - Inputs are implicitly defined
    - Pure Mineral Elastic properties are defined in a database
      - Defined in <external-data>
      - With mandatory columns Young and Poisson
    - Mapping between minerals of the database and geochemical minerals

```
<geoxim-law name="SolidElasticModuliLawConfig">

    <input>
        <rock-volume-fraction>[Phase]Rock::VolumeFraction</rock-
volume-fraction>
    </input>

    <parameters>
        <homogeneisation-method>Voigt</homogeneisation-method>

        <table-poisson-coefficient>0.3</table-poisson-coefficient>
        <table-young-modulus>10.e+9</table-young-modulus>
    </parameters>

</geoxim-law>
```

```
<geoxim-lawname="GeochemicalSolidElasticModuliLawConfig">

  <parameters>
    <homogeneisation-method>VoigtReussHill</homogeneisation-method>

     <mechanical-database>dtbMeca</mechanical-database>

     <mineral-model-mapping>
       <!--Syntax : Mineral: MecaMineral -->
       <map>Calcite:Calcite</map>
       <map>QuartzA:Quartz</map>
      </mineral-model-mapping>

  </parameters>

</geoxim-law>
```


LAWS GEOXIM: ELASTIC PROPERTIES

- System bulk and shear moduli (K, G) knowing (ϕ, K_s, G_s)
  - Hashin-Shtrikman upper bound

$$K(\phi) = \frac{4K_sG_s(1-\phi)}{3K_s\phi+4G_s} \quad G(\phi) = \frac{(1-\phi)G_s(9K_s+8G_s)}{K_s(9+6\phi)+G_s(8+12\phi)}$$

    - Service **HashinShtrinkmanElasticModuliLawConfig**
      - Implicit inputs and outputs
  - Simple Law from Bemer et al 2004

$$K(\phi) = K_s \frac{1}{1+\frac{\alpha_K\phi}{1-\phi}} \qquad G(\phi) = G_s \frac{1}{1+\frac{\alpha_G\phi}{1-\phi}}$$

    - Service **ElasticModuliLawConfig**
      - Implicit inputs and outputs
    - Service **ByZoneElasticModuliLawConfig**
      - Similar with parameters defined by zones

```
<geoxim-law name="HashinShtrinkmanElasticModuliLawConfig">
</geoxim-law>
```

```
<geoxim-law name="ElasticModuliLawConfig">
  <parameters>
    <alpha-bulk>7</alpha-bulk>
    <alpha-shear>12</alpha-shear>
    <max-acceptable-porosity>0.49</ max-acceptable-porosity>
  </parameters>
</geoxim-law
```

```
<geoxim-law name="ByZoneElasticModuliLawConfig">
    <parameter>
      <zonation>[System]System::Facies</zonation>
    </parameter>
    <by-zone-parameters>
      <zone-id>1</zone-id>
       <parameters>
          <alpha-bulk>14</alpha-bulk>
          <alpha-shear>8</alpha-shear>
       </parameters>
    </by-zone-parameters>
    <by-zone-parameters>
      <zone-id>2</zone-id>
      <parameters>
        <alpha-bulk>14</alpha-bulk>
        <alpha-shear>8</alpha-shear>
      </parameters>
    </by-zone-parameters>
</geoxim-law>
```

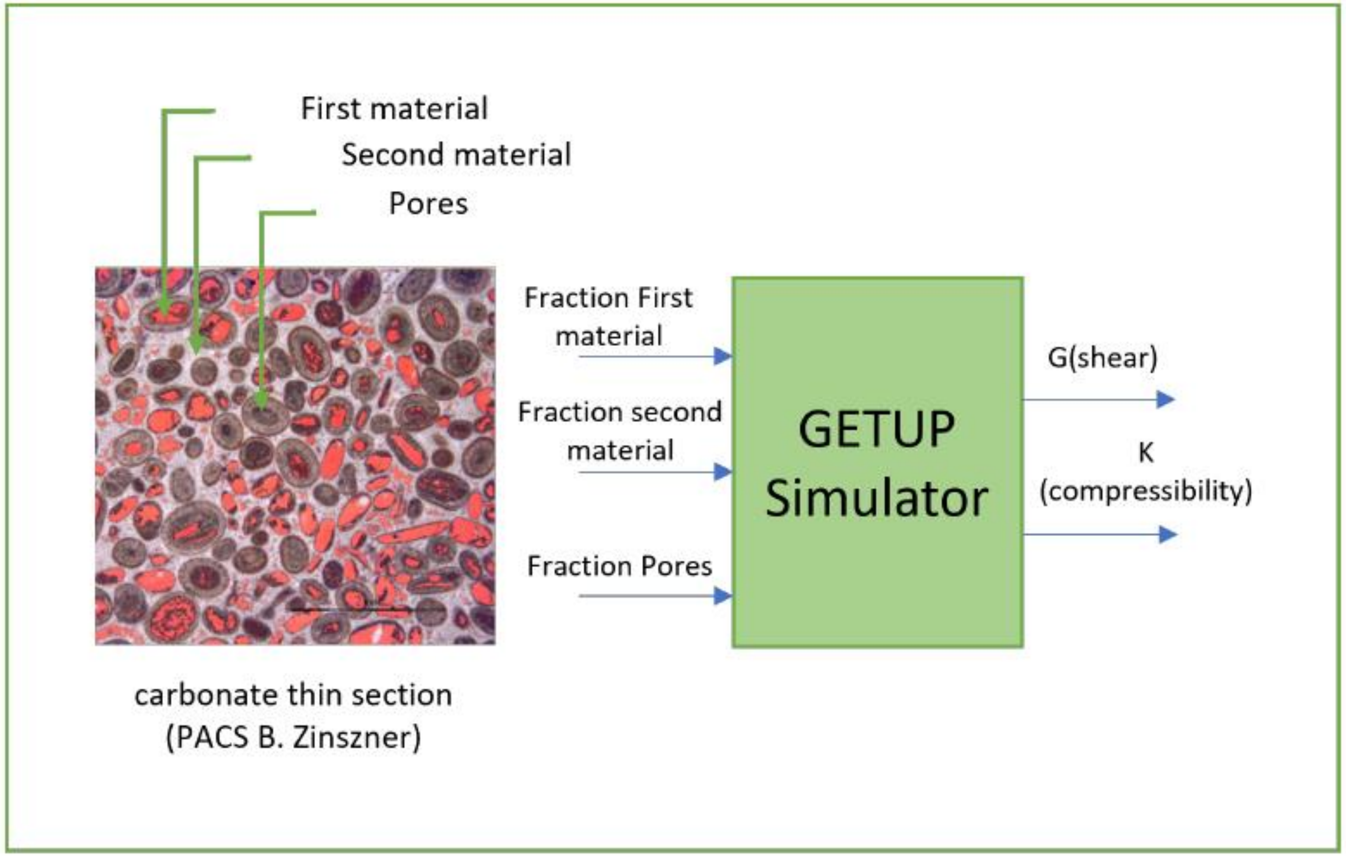

Hashin, Z. 1983. Analysis of composite materials - a survey. Journal of Applied Mechanics. 50: 481–505.

Bemer E., Vincké O., Longuemare P. 2004 Geomechanical Log Deduced from Porosity and Mineralogical Content. OGST 59(4) : 405-426

GETUP

- Intérêt pour les utilisateurs métiers
- Difficile à intégrer comme librairie d'ArcGeoSim
- Evaluation explicite de ces propriétés

GETUP

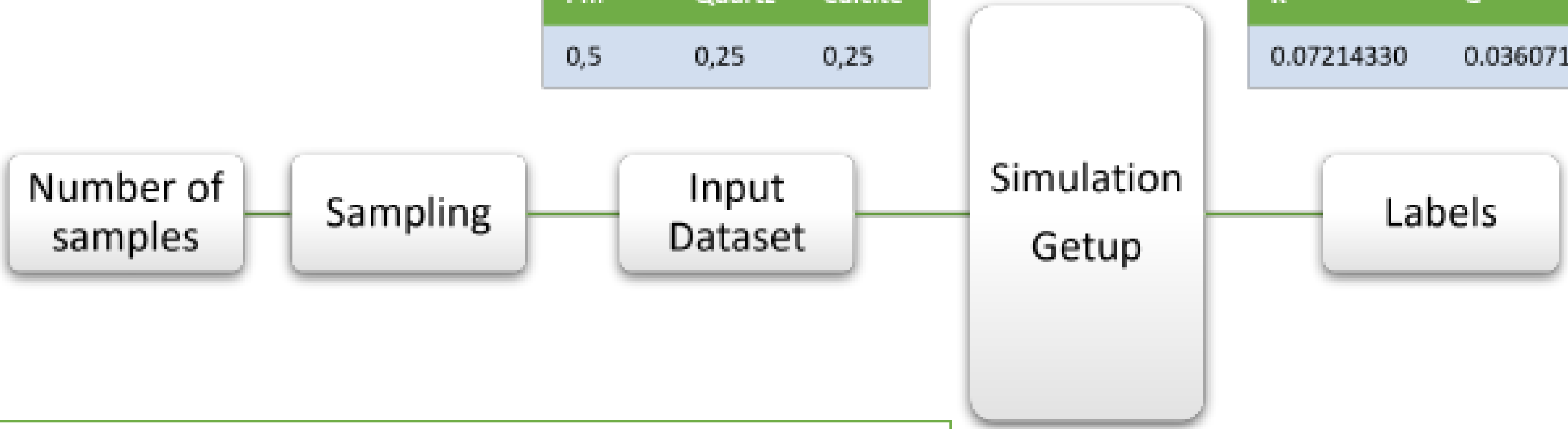


ECHANTILLONNAGE ET DATA SET

Phi in [0,0.5]
Phi+$F_{Quartz} + F_{Calcite} = 1$

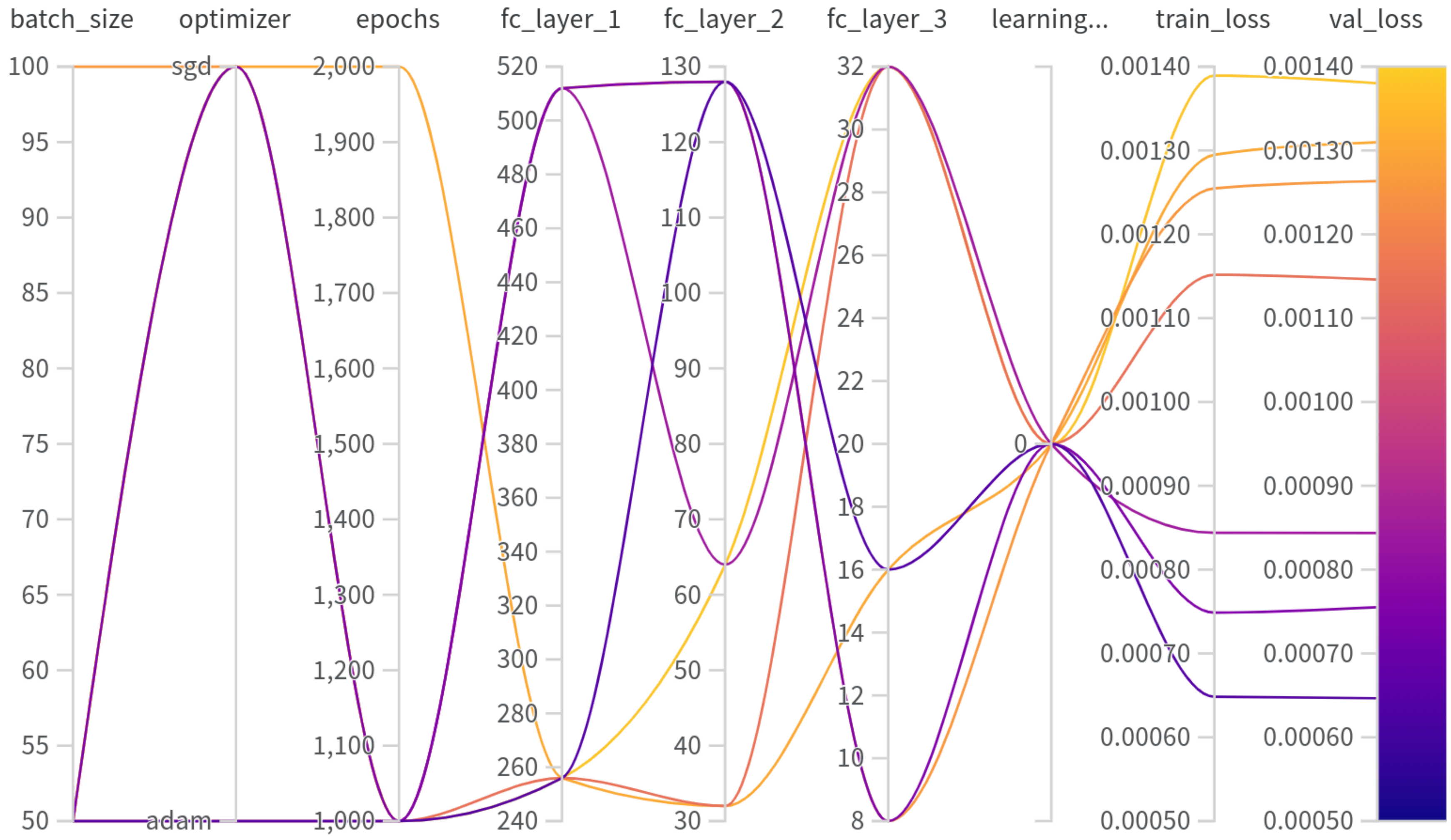
Phi	Quartz	Calcite
0,5	0,25	0,25

K	G
0.07214330	0.03607120



2 Minéraux: Hypercube Latin (100000 échantillons)
6 Minéraux: Dirichlet

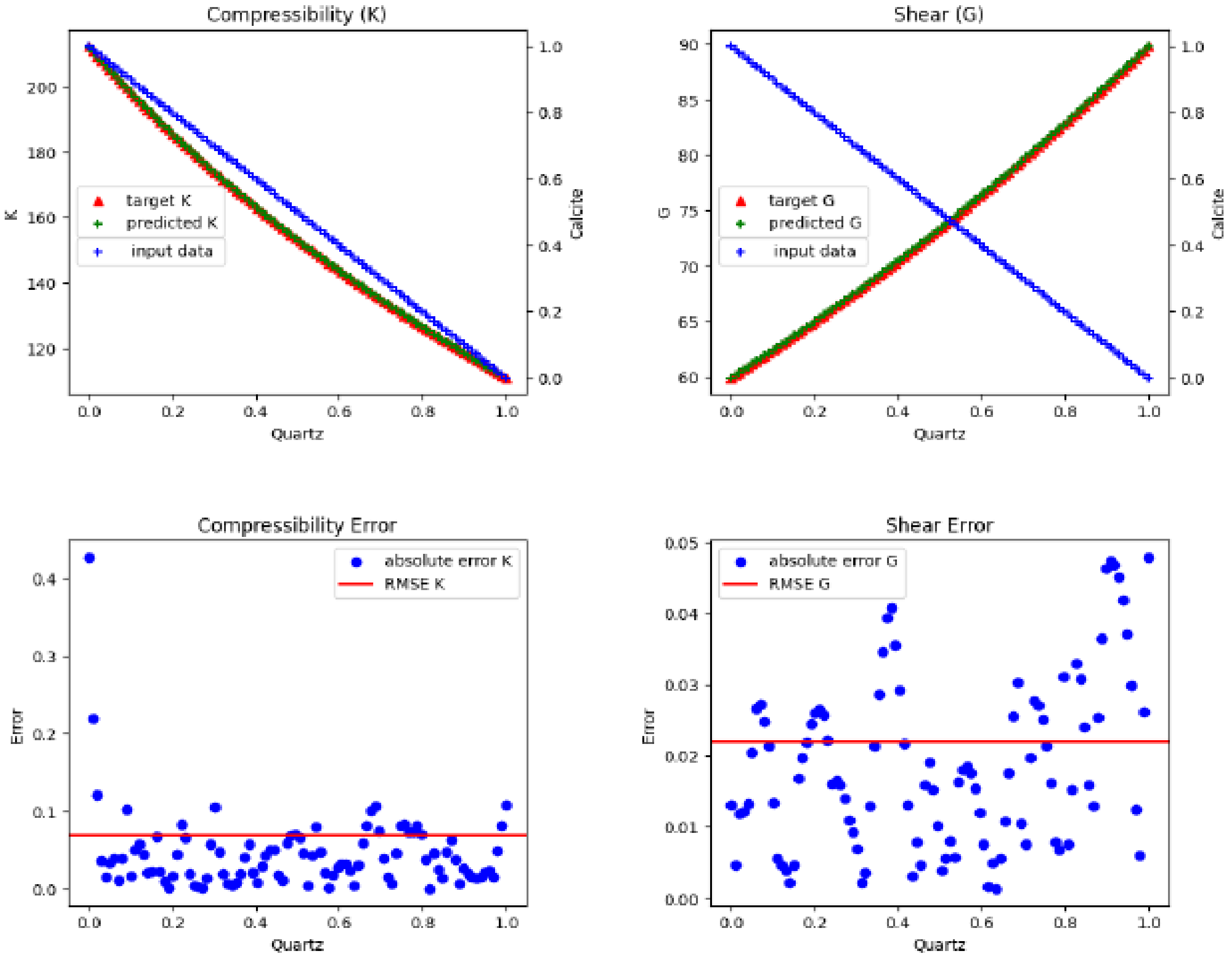
ENTRAINEMENT HYPERPARMETRES 2 MINERAUX



ENTRAINEMENT 2 ET 6 RESEAUX DE NEURONES « GETUP »

Matériaux	Neurones	3 layers	loss_train	loss_val
3	400	[256, 128, 16]	0.0006483	0.0006465
7	256	[64, 128 , 64]	0.1481	0.1497

TEST RESEAUX 3 INPUTS



INFERENCE ONNX DANS LES LOIS

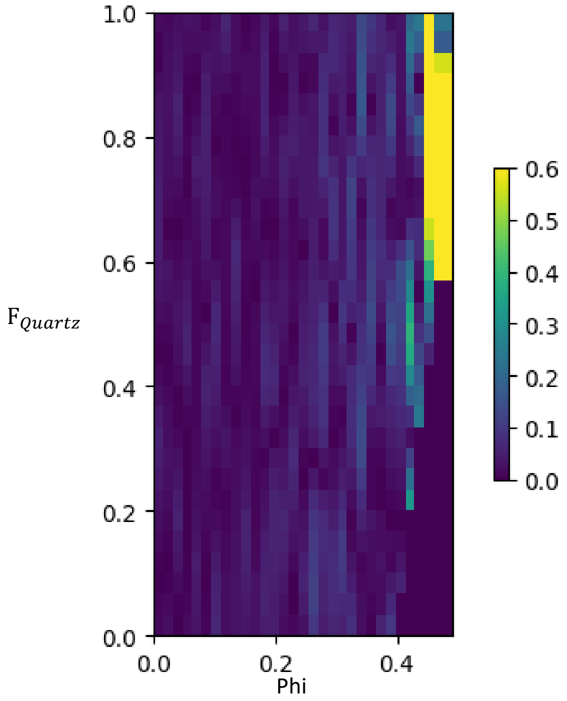
```xml
<makefile>

    <needed-packages>
        <package name="arcane" />
        <package name="onnx" />
    </needed-packages>

    <files language="service">
        <file header="false">OpenNeuralNetworkXLawConfig</file>
    </files>

    <files language="law[inference=onnx]">
        <file>OpenNeuralNetworkXLawType</file>
    </files>

</makefile>
```

config.xml
Compilation time

file .arc
runtime

```xml
<geoxim-law name="OpenNeuralNetworkXLawConfig">
      <onnx-file-name>./model_3_2.onnx</onnx-file-name>
      <outputs>
        <prop-xpath>[System]System::BulkModulus</prop-xpath>
        <prop-xpath>[System]System::ShearModulus</prop-xpath>
      </outputs>
      <inputs>
        <prop-xpath>[SubSystem]Fluid::VolumeFraction</prop-xpath>
        <prop-xpath>[ChemicalPhase]QuartzA::XVolumeFraction</prop-xpath>
        <prop-xpath>[ChemicalPhase]Calcite::XVolumeFraction</prop-xpath>
      </inputs>
 </geoxim-law>
```

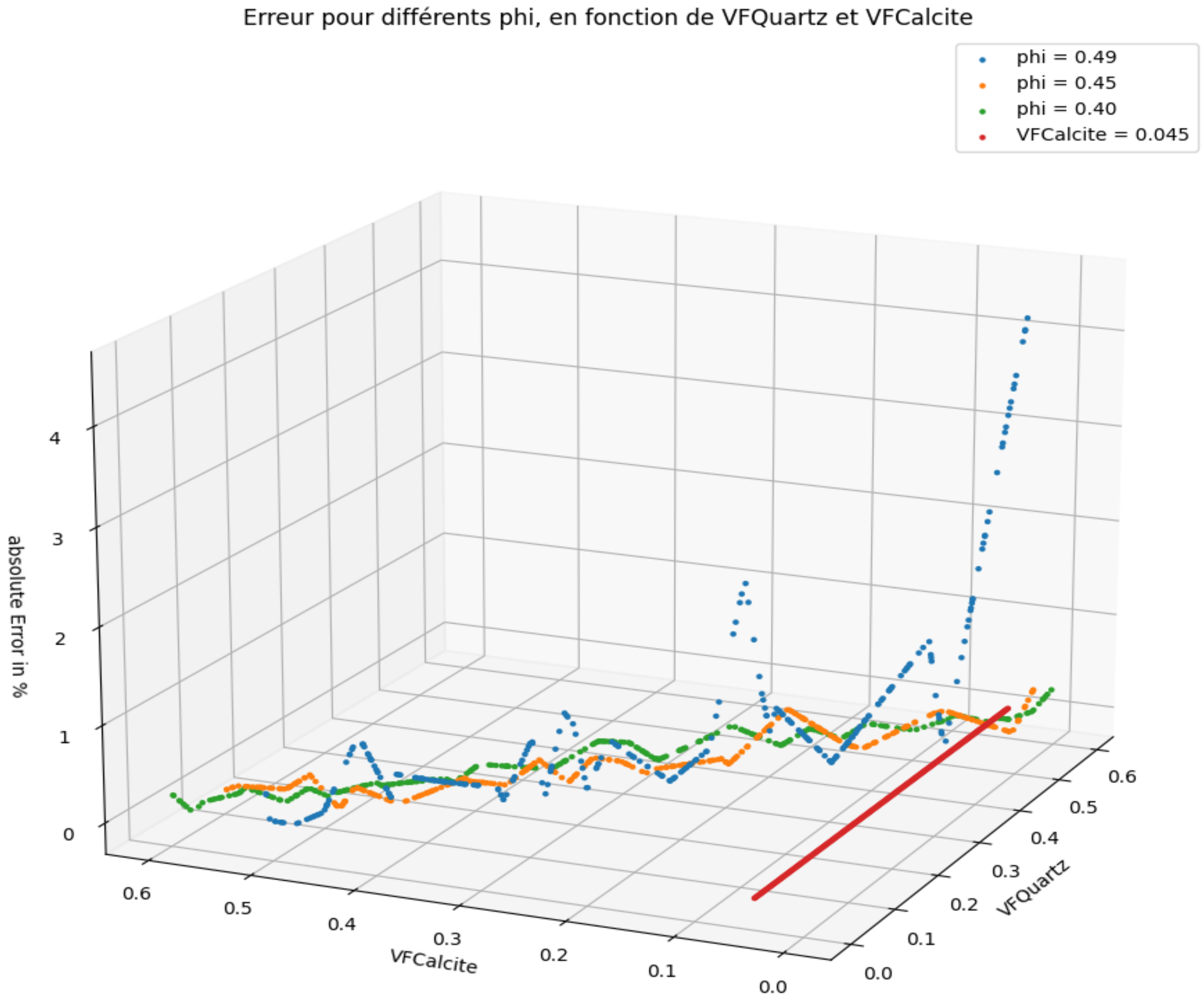
SIMULATION GEOXIM
ERREUR ENTRE UNE TABLE* GETUP ET NOTRE RÉSEAU



	Module d'élasticité (K)	Module de cisaillement (G)
Erreur relative minimale	0.0%	0.0%
Erreur relative moyenne	0,111%	0,089%
Erreur relative maximale	4,360%	3,611%
Ecart type	0,427%	0,323%
Quantile d'ordre 95%	0,225%	0,278%

*table à pas constant de taille 30 x 30
Time in [0.0,0.49] s
F_{Quartz} in [0.45, 0.585] m^3

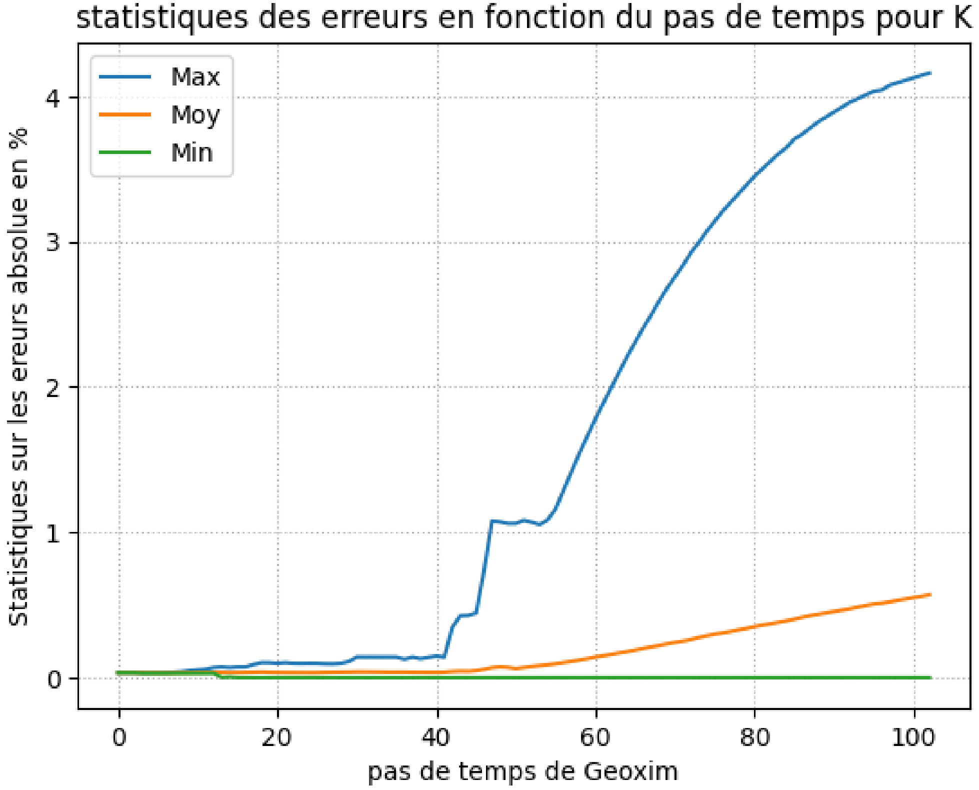
ERREUR RESEAU DE NEURONES A HAUTES POROSITÉS

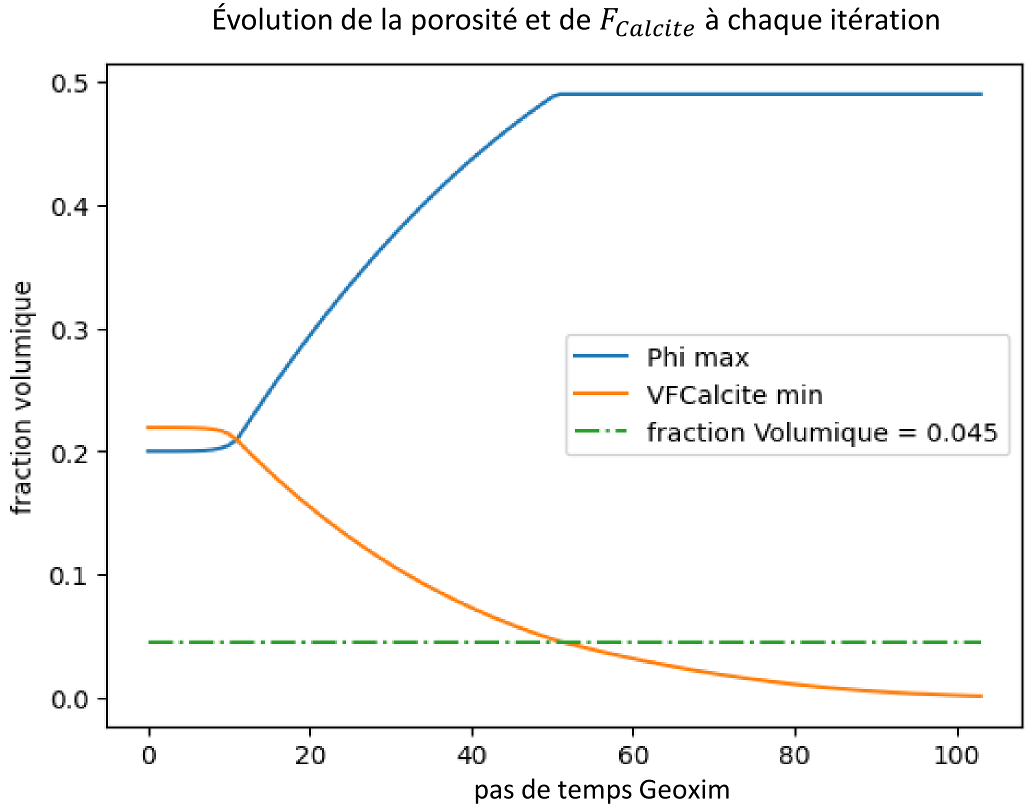


Erreur relative du réseau sur K en fonction de F_{Quartz} $F_{Calcite}$ pour phi ∈ [0.40, 0.45, 0.49]
(Erreur en %)

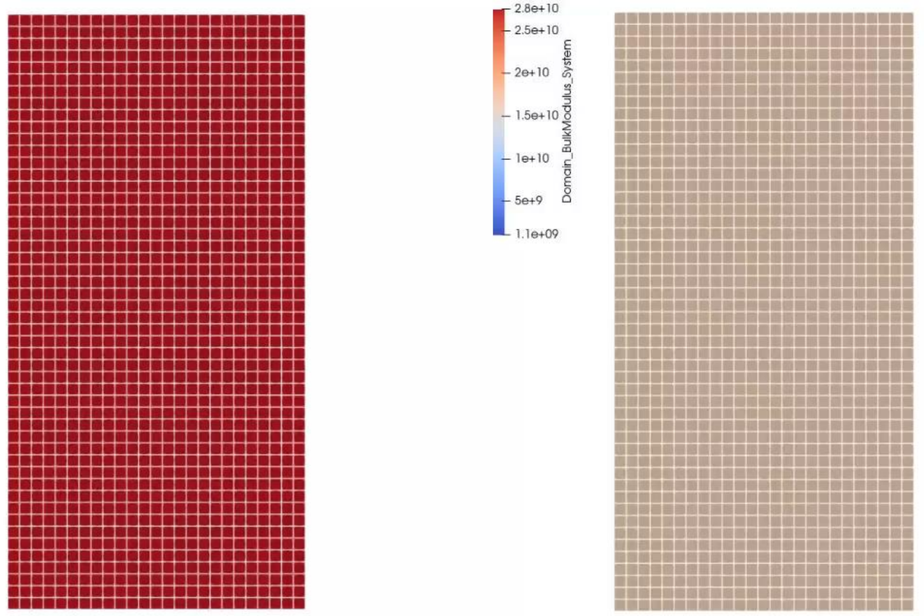
- Erreur sensiblement plus haute à phi = 0.49
- Grande erreur pour $F_{Calcite} < 0.045$

ERREUR RESEAU DE NEURONES AU COURS DE LA SIMULATION GEOXIM

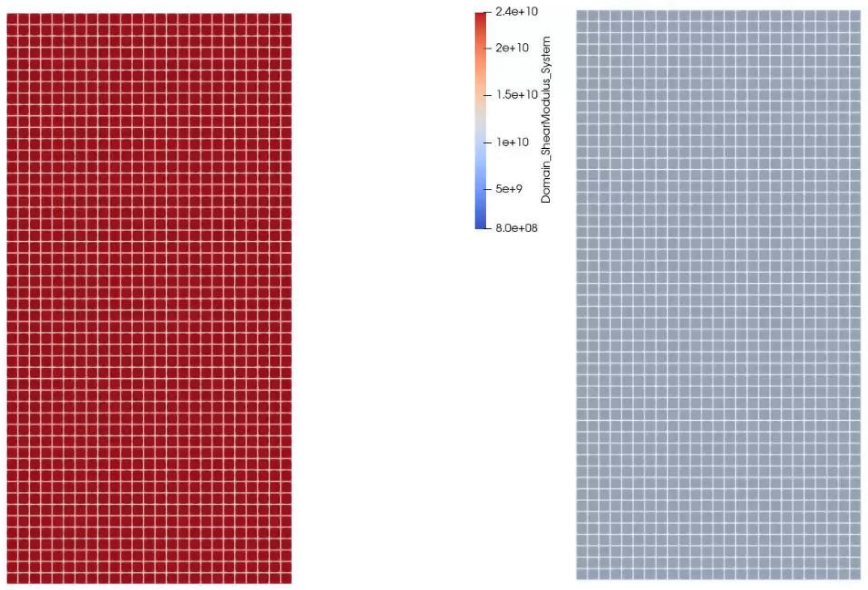




RESULTATS SIMULATION GETUP VS LOIS ANALYTIQES



Différences sur K en fonction
du temps
(incluant le déplacement x80)



Différences sur G en fonction
du temps
(incluant le déplacement x80)

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