SimNet
A Neural Network Based Partial Differential Equation Solver

Release Notes
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### CONFIGURATION:

<table>
<thead>
<tr>
<th>Operating System</th>
<th>• Ubuntu 18.04 or Linux 4.18 kernel</th>
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| Driver & GPU Requirements | • Bare Metal version: NVIDIA driver 465.19 required only if SDF library is used  
 • Docker container: NVIDIA driver 465.19 or higher driver must be used. If using a Tesla (for example, T4 or any other Tesla board), you may use NVIDIA driver release 440.30 or 418.xx however any drivers older than 465 will not support the SDF library. ([https://docs.nvidia.com/deeplearning/frameworks/support-matrix/index.html](https://docs.nvidia.com/deeplearning/frameworks/support-matrix/index.html)) |
|--------------------------|--------------------------------------------------------------------------------|

| Required installations for Bare Metal version | • Python 3.6  
 • Tensorflow 1.15  
 • Horovod 0.21.0 |
|-----------------------------------------------|-------------------------------------------------|

| Supported Processors | • 64-bit x86  
 (this dependency is only when the SDF library is used since the SDF library is compiled on x86. If you need the SDF compiled on Power9 architecture then please e-mail us at: simnet-team@nvidia.com)  
 • NVIDIA GPU based on the following architectures:  
  o Nvidia Ampere GPU Architecture (A100)  
  o Volta (V100, Titan V, Quadro GV100)  
  o Turing (T4, Quadro RTX series)  
  o Pascal (P100, P40, P4, Titan Xp, Titan X) |
|---------------------|-------------------------------------------------------------------------------------------------------------------|

All studies in the User Guide are done using V100 on DGX-1. A100 has also been tested.

**NOTE:** To get the benefits of all the performance improvements (e.g. AMP, multi-GPU scaling, etc.), use the NVIDIA Tensorflow container for SimNet. This container comes with all the prerequisites and dependencies and allows you to get started efficiently with SimNet.
KEY FEATURES – version 21.06 marked as [NEW]:

1. Improved performance with XLA enabled for Tensorflow models and multi-GPU/multi-Node runs:
   a. XLA extensions for Fourier Networks (axis, partial, random & full spectrum)
   b. Strong scaling with learning rate adjustments
2. Improved stability in multi-GPU/multi-Node implementations using linear-exponential learning rate and utilization of TF32 precision for A100 GPUs
3. Physics types:
   a. Linear Elasticity (plane stress, plane strain and 3D)
   b. Fluid Mechanics
   c. Heat Transfer
   d. Coupled Fluid-Thermal [NEW]
   e. Electromagnetics [NEW]
   f. 2D wave propagation [NEW]
4. Solution of differential equations:
   a. Ordinary Differential Equations
   b. Partial Differential Equations
      i. Differential (strong) Form
      ii. Integral (weak) form of the PDEs
5. Several neural network architectures to choose from –
   a. Fully connected Network
   b. Fourier Feature Network
   c. Sinusoidal Representation Network
   d. Modified Fourier Network
   e. Deep Galerkin Method Network
   f. Modified Highway Network
   g. Multiplicative Filter Networks [NEW]
6. Features include –
   a. Global mass balance constraints
   b. SDF (Signed Distance Function) weighting of PDEs in flow problems for rapid convergence
   c. Exact mass balance constraints
   d. Global and local learning rate annealing
   e. Global adaptive activation functions
   f. Halton sequences for low-discrepancy point cloud creation
   g. Gradient Accumulation [NEW]
   h. Time-stepping schemes for transient problems [NEW]
      i. Temporal loss weighting and time marching for the continuous time approach [NEW]
      j. Importance sampling [NEW]
   k. Homoscedastic task uncertainty quantification for loss weighting [NEW]
7. Parameterized system representation that solves several configurations concurrently for analytical geometry using SimNet CSG module
8. Transfer learning for efficient surrogate-based parameterization of STL and constructive solid geometries [NEW]
9. Polynomial Chaos Expansion method for assessing how uncertainties in a model input manifest in its output [NEW]

10. APIs to automatically generate point clouds from Boolean compositions of geometry primitives or import point cloud for complex geometry (e.g., STL files)

11. Geometry library to either construct point cloud using simple primitives or from an STL using superfast ray tracing method with uniformly emanating rays using Fibonacci sphere. Point categorized as inside, outside or on-the-surface, SDF and its derivative calculation. Implementation of new technique for more accurate and faster SDF calculation

12. Logically separate APIs for physics, boundary conditions and geometry consistent with traditional solver datasets

13. Step by step tutorials for getting started with:
   a. computational fluid dynamics
   b. zero-equation turbulence model
   c. heat transfer
   d. inverse problems and multi-physics problems

Known issues:
1. It is known that sometimes Horovod prints numerous warning messages of this type:
   ```
   Read -1, expected xyz, errno = 1
   ```
   These messages are harmless and can be filtered out by using the below command:
   ```
   horovodrun <#GPUs> python <script.py> |& grep -v "Read -1"
   ```

2. It is known that sometimes Horovod gives multiple stalled or missing rank warnings, and in most cases these prevent the training to start. We have observed that by reducing the GPU memory usage (e.g., reducing the batch size), this issue can be fixed.