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EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN **SCIENTIFIC COMPUTING**

MULTI-GPUS IMPLEMENTATION WITH GRAPH NEURAL NETWORK TO SOLVE SPARSE LINEAR SYSTEMS FOR MASSIVE COMPUTATIONAL PROBLEMS

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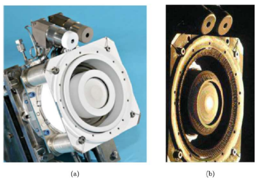
Motivation for Hall-Effect Thruster (HET) Numerical Simulation with Machine Learning (ML)

Modeling plasma numerical simulations:

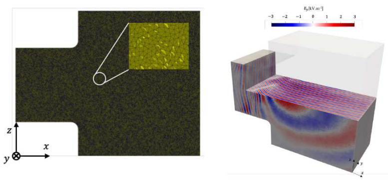
- Tracking instabilities for HET experimental design.
- **BUT** expensive due to **Electric Field** computation.



HETs : (a) PPS-1350 and (b) PPS-1350 severely eroded (Credits Safran)

Objective → Speed Up the resolution of Poisson equation.
Method → Coupling traditional methods and ML.

3D Particle-In-Cell PIC simulation of HET over 15 million elements for unstructured mesh.



Electric Field computation

- Need to solve Poisson equation to get the electric field for plasma modeling

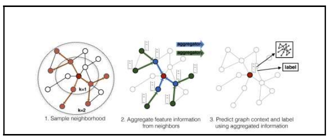
$$\Delta\Phi = -\frac{\rho}{\epsilon_0}$$

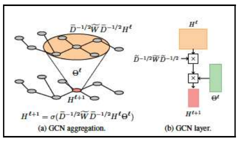
- Discretization of Poisson equation into a linear system $\mathbf{A}.\mathbf{x} = \mathbf{b}$ for unstructured mesh.
- Coupling iterative solvers, e.g. **G**eneral **M**inimal **RES**idual (**GMRES**), or **C**onjugate **G**radient (**CG**) and using neural networks as preconditioners to get the solution of linear systems faster.

Graph Neural Network (GNN)

Spatial Graph Convolution [1]

- Supervised or Semi-supervised learning [2] for geometric problems → $H^{l+1}(\Theta)$ with (W, D), geometric values of the GNN.
- Output GNN: $H^{l+1} = \sigma(g_1(W,D)\,H^l\,\Theta_1 + g_2(W,D)\,H^l\,\Theta_2)$





GraphSage from Hamilton *et al.* and aggregation scheme for Graph Convolutional Network (GCN)

ELISA Framework to solve Poisson equation

ELISA (**E**nhanced **L**inear **I**terative **S**olver with **A**rtificial intelligence)

- Framework based on Pytorch Geometric and Pytorch for image or graph learning.
- Distributed Data Parallelism paradigm.
- Bayesian Neural Networks (BNNs) for Uncertainty Quantification.

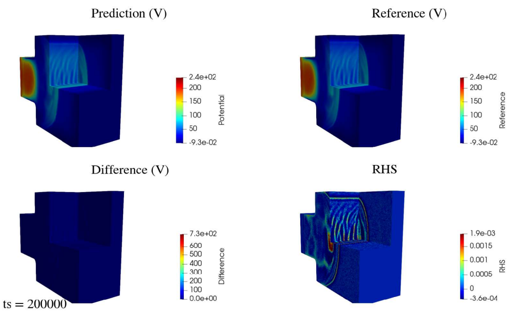
Training Procedure with ELISA:

Get the number of unknowns for the linear system n_{eq}
Initialize input_data array of neural network input_data$[n_{eq}, 2]$
for $i \in 1, ..., t$ **do**
  input_data$[:, 0] = u_{i-1}$
  input_data$[:, 1] = \mathbf{Fp}_i$
  $u_i \leftarrow u_{i-1} + f_\theta(u_{i-1}, \mathbf{Fp}_i)$
  $\mathcal{L}_\theta \leftarrow ||\mathbf{A}.u_i - \mathbf{Fp}_i|| + \frac{1}{n_{eq}}\sum_{i=1}^{n_{eq}}(u_i - u_{i,ref})^2$ ▷ L2 residual norm + MSE
  $\theta \leftarrow \text{ADAM}(\theta, \nabla_\theta\mathcal{L}_\theta)$ ▷ Update Parameters with ADAM
  $u_i \leftarrow \text{GMRES}(u_i)$ ▷ new *input_data*$[:, 0]$ for next timestep
end for

Semi-supervised learning to solve linear system coupled with iterative solver (i.e. GMES)

Results for Graph Neural Network coupled with iterative solvers

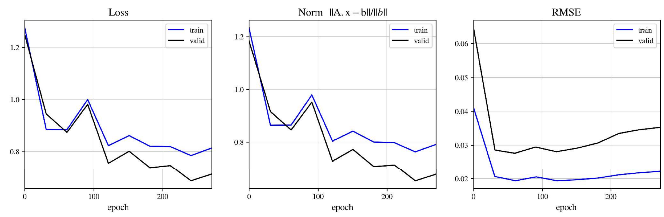
- Capability to make training and inference on very large graphs.
- Methodology to generalize the resolution of linear systems.



Inference for the training set for a massive plasma simulation problem

Final Requirements:

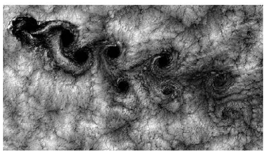
- Reduce the computation time by a factor of **5** to **10**.
- Extend the learning process **for all linear systems** with different geometries (structured or unstructured mesh, 2D or 3D).
- Reach of tolerance level of 10^{-2} for each linear system.



Inference for training and validation set for a Finite-Element Method Plasma Simulation

Prospects

- Solving Poisson equation for incompressible Navier-Stokes: $\Delta^2\mathbf{p}^{n+1} = \rho\frac{\nabla.\mathbf{u}^n}{\Delta t} - \rho\nabla.(\mathbf{u}^n.\nabla\mathbf{u}^n) + \mu\nabla^2(\nabla.\mathbf{u}^n)$
- Solving Helmholtz equation for wave propagation problem: $\left[\nabla^2 + \left(\frac{\omega}{c(r)}\right)^2\right]\mathbf{u}(r) = \rho(r)$



References

[1] William L. Hamilton *et al.*, *Inductive Representation Learning on Large Graphs*, 2018,

[2] Sami Abu-El-Haija *et al. MixHop: Higher-order graph convolutional architectures via sparsified neighborhood mixing.*. ICML, pages 21–29, 2019

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