Meta-Programming and Hybrid Parallel Strategies for Solving PDEs: An FDM and PINN Comparison [1] [2]

Seminar Presentation III

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[1] full docs: `https://liyihai.com/html/index.html`

[2] repository: `https://github.com/liyihai-official/Final-Project`

Outline

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Kolmogorov PDEs

Solving $u(x,T)$, for $\mathbb{R}^1 \ni T > 0$, $x \in \mathbb{R}^d$, $t \in [0,T]$, $u(t,x) = u \in \mathbb{R}^1$, $\mu(x) \in \mathbb{R}^d$, $\sigma(x) \in \mathbb{R}^{d\times d}$,

$$u_t = \frac{1}{2}\,\mathrm{Trace}_{\mathbb{R}^d}\left[\sigma(x)\,[\sigma(x)]^*\,\mathrm{Hess}_x u\right] + \langle \mu(x), \nabla_x u\rangle_{\mathbb{R}^d} \tag{1}$$

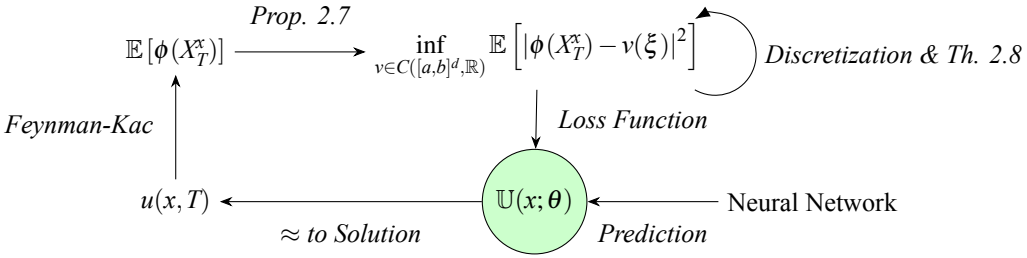

Figure: Deep Neural Network (DNN) Methodology of Solving Kolmogorov PDEs [**FIRST**]

General Form of PDEs

– $u(t,x)$ denotes with the target function, $x \in \mathbb{R}^d$.

– $\Gamma[\,\cdot\,;\lambda]$ is a non-linear operator parameterized by λ.

$$u_t(t,x) + \Gamma[u;\lambda] = 0 \tag{2}$$

Define $f(t,x)$ to be given by

$$f(t,x) = u_t(t,x) + \Gamma[u;\lambda] \tag{3}$$

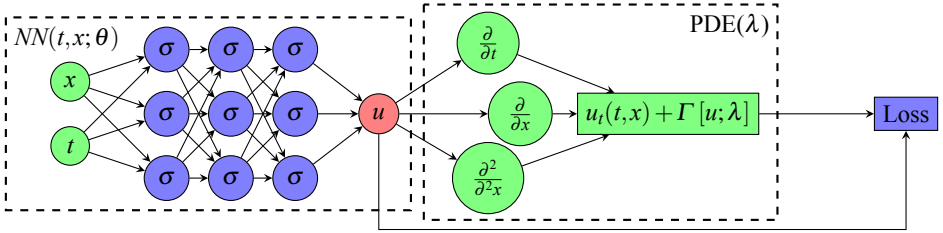

Figure: PINN, with with 3 fully connected hidden layers

Comparing With Finite Difference Time Domain Method (FDTD)

1. Deep Neural Network [**FIRST**]
   - Gives lower quality approximations.
   - Takes longer time to train.
   - Possible to solve high dimension PDEs
2. Physics Informed Neural Network
   - Gives higher quality approximations.
   - Takes longer time to train.
   - Has more flexible way to get results.
   - Possible to solve high dimension PDEs

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General Form of problem

The PDE parametrized by number λ and an operator $\mathscr{N}[\cdot;\lambda]$, and assume the variable x is a 2D or 3D spatio-vector which is written in

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,\vec{x}) + \mathscr{N}[u;\lambda] = 0 \\ u(0,\vec{x}) = \varphi(\vec{x}) \end{cases} \tag{4}$$

where φ is the initial condition, and $\vec{x} \in \Omega, t \in [0,+\infty)$.

Boundary Conditions

The Dirichlet and Von Neurmann boundary conditions are formed as

$$\begin{cases} u(t,\vec{x}) = g(t,\vec{x}) \\ \dfrac{\partial u}{\partial \vec{n}} = g(t,\vec{x}) \end{cases} \tag{5}$$

where $\vec{n}$ is the normal vector on $\overline{\Omega}$ the boundary of domain Ω.

Heat Equation 2D

The function $u(t,x,y) = x+y-xy, \forall \alpha \in \mathbb{R}^1$, is the solution of 2D Heat Equation 6 below

$$
\begin{aligned}
&\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial u^2}{\partial^2 x} + \frac{\partial u^2}{\partial^2 y} \right) && (x,y) \in \Omega,\ t \in [0,+\infty) \\
&u(0,x,y) = \varphi(x,y) = 0 && (x,y) \in \Omega \\
&u(t,x,y) = g(x,y) = \begin{cases} y,\ x = 0, y \in (0,1) \\ 1,\ x = 1, y \in (0,1) \\ x,\ y = 0, x \in (0,1) \\ 1,\ y = 1, x \in (0,1) \end{cases} && t \in [0,+\infty)
\end{aligned}
\tag{6}
$$

Heat Equation 3D

The function $u(t,x,y,z) = x+y+z-2xy-2xz-2yz+4xyz, \forall \alpha \in \mathbb{R}^1$, is the solution of 3D Heat Equation 7 below

$$
\begin{aligned}
&\frac{\partial u}{\partial t} = \alpha\left(\frac{\partial u^2}{\partial^2 x}+\frac{\partial u^2}{\partial^2 y}+\frac{\partial u^2}{\partial^2 z}\right) && (x,y,z)\in\Omega,\ t\in[0,+\infty)\\
&u(0,x,y,z) = \varphi(x,y,z) = 0 && (x,y,z)\in\Omega \qquad (7)\\
&u(t,x,y,z) = g(x,y,z) = \begin{cases} y+z-2yz, & x=0,\\ 1-y-z+2yz, & x=1,\\ x+z-2xz, & y=0,\\ 1-x-z+2xz, & y=1,\\ x+y-2xy, & z=0,\\ 1-x-y+2xy, & z=1 \end{cases} && t\in[0,+\infty)
\end{aligned}
$$

Challanges of Nonlinear Multi-Scale Systems

1. Difficulty in modeling and predicting inhomogeneous cascades of scales.
2. High computational costs and uncertainties in classical methods.

Project Objectives

1. Implement FDTD and PINN in `C++/C`.
2. Implement FDTD hybrid parallel version using `MPI/OpenMP`.
3. Implement PINN GPU parallel version using `Libtorch/CUDA`.
4. Optimize performance through parallel computing frameworks.
5. Evaluate the efficiency and accuracy of FDTDs and PINNs.

Highlights

Outline

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Closing Remarks

Thank you for your attention!

Any questions?