Using QPINNs in Climate Change Modelling

Team Kickoff Meeting

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Meet the Team – Introduce Yourselves

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Some Rules

1. Please be respectful of everyone (your team members, GGRP staff, fellow participants, etc.) at all times irrespective of their culture, ethnicity, country of origin, religion, gender identification, etc.
2. We are all aware of what's going on in the world right now: Wars, riots, dissent against governments, etc. Please, this group is neither the platform, and this programme is nor the place, to discuss this. Let's strive to be professional, and become better Scientists.
3. Please be punctual for meetings, and do not spam groups with irrelevant posts / messages.
4. Please honour your commitments to deliver work, and deliver work that is of high quality in a timeous manner.
5. Strictly, no plagiarism, and copying and pasting from ChatGPT, etc.
6. Please do not share links to our papers, code, or any material with anyone outside of our team!
7. Please respect all edicts you've signed up for in the GGRP, and do not participate in any illegal activities.

Why is this Project Beneficial for you?

- To teach you how to go about doing research, and give you a flavour of all that comes along with it.
- Climate change is a hot topic right now! So it ML! Thus, by combining the two, you gain valuable research skills, and have solid grounds for attracting funding for graduate school research.
- Having a published research paper on your resume looks really good, especially if you want to pursue a career in a research lab, like DeepMind or FAIR, or want to study further – Trust me it really helps your graduate school applications.
- Makes for a cool LinkedIn post!

What is Climate Change?

The alteration of weather conditions such as global temperatures, sea levels, changing levels of precipitation (rainfall), that has a lasting and disastrous affect on our planet.

- There is a big drive by governments, the UN, the IPCC, the WHO, presidential bodies and special committees, etc. to try and curb climate change. Thus, big money for anyone / organisation that can make some impact!
- The foremost driver behind climate change is industrialisation, and human activities that release greenhouse gases such as CO_2, CH_4, and N_2O. These gases get trapped in the atmosphere, and increase the global temperature over time.

Impacts of Climate Change

- Rising global temperatures.
- Abnormal precipitation patterns which results in flash floods, storms, droughts, and other extreme weather conditions.
- Melting glaciers and polar ice caps which result in rising sea levels. This results in coastal erosion, lose of global landmass and islands, and even cities (apparently Venice is sinking).
- Disruption of natural ecosystems. This results in decrease in population numbers, and oftentimes complete obliteration, of plant and animal life.
- Impact on human beings – Health related issues, airborne diseases, etc.

Why is Combating Climate Change Important?

1. Safeguarding biodiversity and the environment.
2. Safeguarding human health.
3. Ensuring food security for all people.
4. Curbing risks associated with the economic implications.

And many many more.

Equations of Climate Change Which We Will Attempt to Solve

1. **Geostrophic Motion:** Movement of a fluid (air or water) in the atmosphere. It occurs at low Rossby number ($\varepsilon = U/2\Omega L$), where U is the characteristic speed relative to the earth, Ω is the angular speed of the earth, and L is a characteristic length. In $\mathbb{R}^3$, it is given by

$$\begin{aligned} -2\Omega u &= -\frac{1}{\rho}\frac{\partial p}{\partial x} \\ 2\Omega v &= -\frac{1}{\rho}\frac{\partial p}{\partial y} \\ \frac{\partial p}{\partial z} &= -\rho g, \end{aligned}$$

where $p = p(x, y, z)$, or in compact vector form $\mathbf{f} \cdot \mathbf{v} = -\frac{1}{\rho}\boldsymbol{\nabla} p(x, y, z)$.

2. **Shallow Water Wave Equation:** Describes the behaviour of waves in shallow water. Mathematically,

$$\frac{\partial^2 h}{\partial t^2} + c^2 \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right) = 0,$$

where $h(x, y, t)$ is the surface elevation of water above a reference level, c is the wave speed.

3. **The Sea-Ice-Thickness Model:** We model the ice-thickness field, $H(\mathbf{x}, t)$, and meltwater pond depth, $w(\mathbf{x}, t)$ as

$$\begin{aligned} \frac{\partial H}{\partial t} &= -f(H, w), \\ \frac{\partial w}{\partial t} &= -\boldsymbol{\nabla} \cdot (\mathbf{u} w) + \frac{\rho_{\text{ice}}}{\rho_{\text{meltwater}}} f - s(H, w), \end{aligned}$$

where f is the melting rate, s is the seepage rate, and $\mathbf{u}w$ is the meltwater flux (flow per cross-sectional area, per unit time).

4. If time permits, we can explore the control of an invasive species model, governed by dynamical systems.

What are PINNs?

- *Physics-Informed Neural Networks* (PINNs) are a supervised learning ML algorithm that combines data and the constraints imposed by the physics of a scenario to solve the underlying differential equations that govern the system under study.
- Given a system Ω with varying quantities $\mathbf{u} = \langle u_1(t, \mathbf{x}), u_2(t, \mathbf{x}), \ldots, u_n(t, \mathbf{x}) \rangle$ that possess the governing system of equations

$$f\left(\frac{\partial \mathbf{u}}{\partial t}, \frac{\partial^2 \mathbf{u}}{\partial t^2}, \ldots, \frac{\partial \mathbf{u}}{\partial \mathbf{x}}, \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2}, \ldots\right) = 0,$$

where $\mathbf{x} = \langle x_1, x_2, \ldots, x_m \rangle$ are the spatial variables, having loss function

$$\mathcal{L}_{\text{physics}} = \frac{1}{N} \sum_{i=1}^{N} |f|^2,$$

where N is the number of data points, and data loss $\mathcal{L}_{\text{data}}$, we write a combined loss function

$$\mathcal{L} = \mathcal{L}_{\text{physics}} + \lambda \mathcal{L}_{\text{data}},$$

where $\lambda \in (0, 1)$ is a hyperparameter.

- The loss function is minimised in order to determine the optimal weights, which are found found using gradient descent

$$\mathbf{w} \longleftarrow \mathbf{w} - \alpha \boldsymbol{\nabla}_{\mathbf{w}} \mathcal{L},$$

where α is the learning rate / step size.

- The data is obtained by sampling from the domain of interest. Oftentimes, if data is unavailable, it is synthetically created, and then sampled from.
- The loss function for the data is the data MSE loss, or any other variant,

$$\mathcal{L}_{\text{data}} = \frac{1}{M} \sum_{i=1}^{M} |u_i(t, \mathbf{x}) - \hat{u}_i(t, \mathbf{x})|^2,$$

where M is the number of datapoints.

What are QPINNs?

- Essentially, the quantum version of classical PINNs.
- They are useful because they can potentially offer a quicker way to compute gradients, and solve the underlying governing PDEs due to superposition of states.
- Additionally, QPINN algorithms may be less computationally expensive and may be easier to implement.
- I'm hoping you can tell me, and teach me more!

Recommend Readings and Literature Papers

1. Cai, S., Mao, Z., Wang, Z., Yin, M., & Karniadakis, G. E. (2021). *PINNs for Fluid Mechanics: A Review*. Acta Mech. Sin. pp. 1727-1738, https://arxiv.org/pdf/2105.09506.pdf.
2. de Wolff, T., Carrillo, H., Marti., L., & Sánchez-Pi, N. (2021). *Assessing Physics Informed Neural Networks in Ocean Modelling and Climate Change Applications*, https://inria.hal.science/hal-03262684/.
3. "...", *Towards Optimally Weighted PINNs in Ocean Modelling*, https://arxiv.org/pdf/2106.08747.pdf.
4. QPINNs: https://www.frontiersin.org/articles/10.3389/fams.2022.1036711/full
5. QPINNs: https://arxiv.org/pdf/2304.11247.pdf

Project Plan

In order to get a preprint, and hopefully a fully published paper, we will start writing from the beginning.

- The link to the research paper for this project is: https://www.overleaf.com/4455198112nhzntdxhkjwn#1796af.
- The link to our GitHub is: https://github.com/MuhammadAlZafarKhan/QPINNs-for-Climate-Change.
- We will run the programme on a lean 8-week cycle, with weekly check-ins, and *occasional* check-ins during the course of each week – Might be through Discord, or if the need arises, the calling up of a meeting.
- **Note:** We will use American English in writing papers, presentations, etc. in order to keep abreast with international standards.

- **Week 1:** Familiarise yourselves with the underlying material, and start writing up the Introduction, and Literature Review, based on your readings, while it's still fresh in your mind.
- **Week 2:** Continuation and completion of initial Introduction and Literature Review (we will gradually add to, and remove stuff as we go along), and write-up of the Theory aspect of the paper.
- **Weeks 3-6:** Completion of the Theory, starting and completion of any experiments.
- **Week 7:** Writing up of Conclusion, and touch-ups to the paper. Thereafter, submission to arXiv, and maybe, depending in the quality of the results, to a journal / conference (we will discuss which journal as time progresses).
- **Week 8:** Creating a presentation on the work we've done, lessons learned, and practice delivering the presentation.

The End

Questions?