Paper-1. 6/09/23 Machine Learning and Quantum Computing for Reactive Turbulence (2021) Modeling and Simulation - Peyman Givi

ref: 13th Elsevier Distinguished Lecture in Mechanics

QIS.

ML - vision, autonomous systems and NLP.

Supervised, totally data driven ML

Deep learning via neural networks - complex classifications and regression tasks.

PSciences → construct predictive models of complex physical systems

QIS: - Quantum physics & Information Technology

Quantum algorithms - Shor's algo

↓

factorisation of integers

Grover's algorithm:- unstructured search problems

Gain in efficiency - These can be exponential or polynomial.

~~"as quantum~~ "quantum speed-up"

Applican in Reactive Turbulence!

↓ unresolved problem

↓ significant scientific and practical applican

length and time ↓ broad range ↓ computational descripn is difficult

ML

ML optimisation Techniques

magneto hydro dynamics
MHD?

RANS (Reynolds - averaged Navier - Stokes)

turbulent electro magnetic fields?

LES (Large Eddy Simulation)

→ solar corona??

coherent vs. stochastic structures, - γ(flow) (Hydrodynamic stability?)

linear vs non linear physics

small changes in initial can lead to large changes in final outcome

eg: turbulent fluids, chaotic systems and complex networks

issues pertaining to ML application in reactive turbulence modelings:-

1) Amount, Quality and Complexity of Data.

→ accuracy target.

→ combustion turbulence

flow data sets :- Sandia TNF Workshop (tnfworkshop.org)

2) physics discovery: reconstruct modelled transport equations

"non-autonomous dynamical systems"

→ recover symmetries including invariances.

→ "reinforcement learning" strategy optimization" leo dynamics

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* Inverse & Ill posed problems:-
> Doesn't meet Hadamard criteria of being well posed

Similarities and commonalities: non-linear dimensional reductions for large volume

* Auto differentiation could enable efficient analysis of simulation results.

Quantum computing: Not the next step, but a whole new journey

domain driven & data driven models

ML - must be utilised in the context of very strong domain modeling

Perspectives of QC

quantum advantage over classical is achieved if
↑se qubits to about 50 & ↓se error rate to less than 0.1%.

* Solution of multi-dimensional non-linear partial differential equations as required for turbulent combustion computations on a digital universal quantum computer would require a fault-tolerant computer along with millions of gates and qubits. *

It'll take decade

near-term alternatives :-

1) NISQ : Noisy Intermediate-scale Quantum
↳ without any quantum error correction
ML, optimisation, chemistry, material science etc applica?

2) Analog Computers, Quantum simulators and Annealers :
→ Quantum speedups
→ Continuously in time rather than being broken into discrete quantum gates.
→ D wave computers.

3) Hybrid Quantum-classical computing : (HQCC)
co-processor → combines power of classical and quantum computers to compute faster

4) Quantum Algorithms ~~that~~ :- Identifying classical
Inspired algorithms that are
• Quantum Inspired [3]

eg: MPS [matrix product state) → large scale turbulence simulations yplica?

into

MPS:- sub type of tensor networks. It works by mapping
the differential equations (~~NS~~ Navier-Stokes, reaction
diffusion, energy etc) onto a tensor network, and evolving
the tensor network towards solution.

→ strongly correlated quantum systems

** "Tensor Network Theory" **