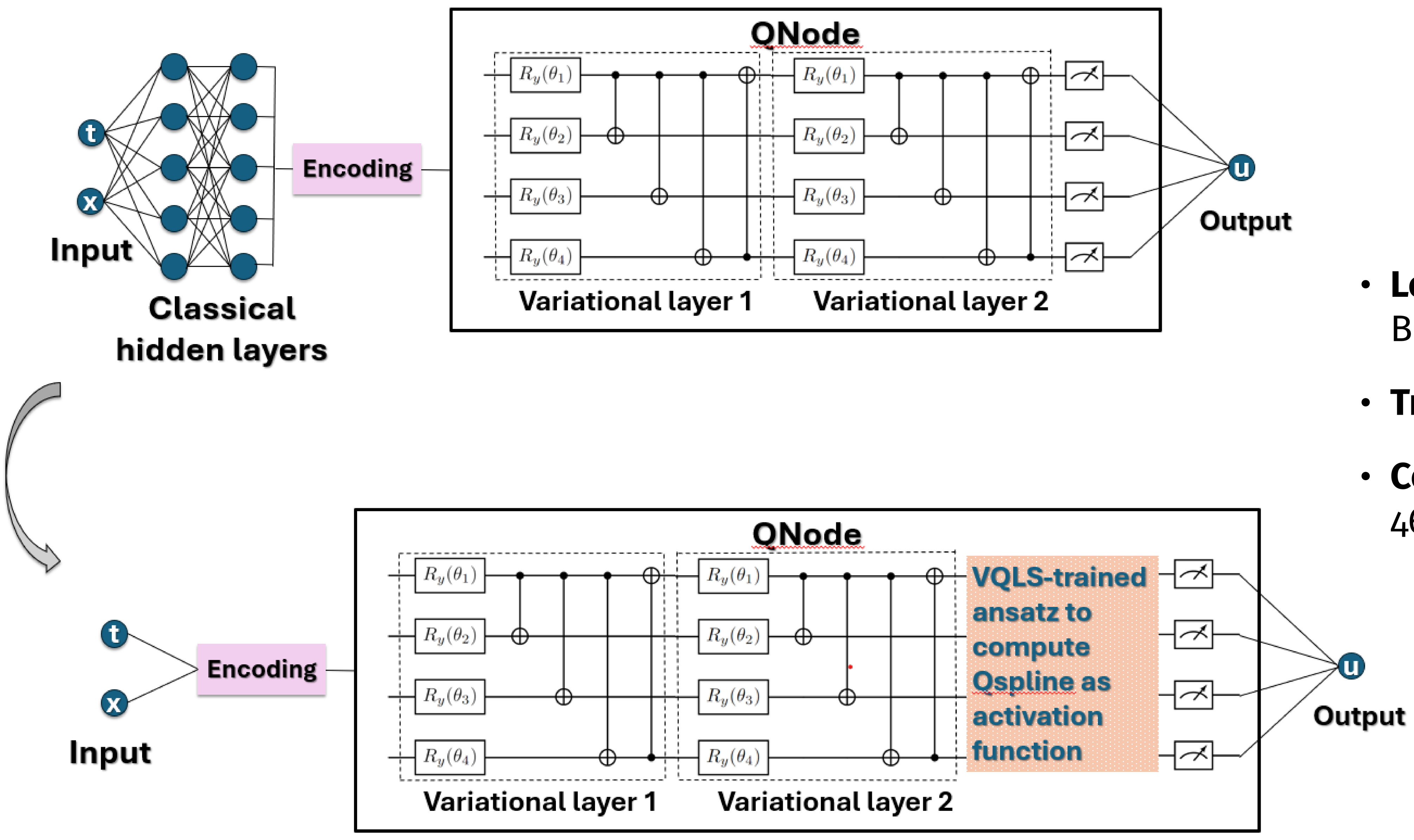
Nonlinear Activation using Variational Quantum Splines in Quantum Physics Informed Neural Networks

Apurva Tiwari Jay Pathak
Ansys Inc., India/U.S.A.

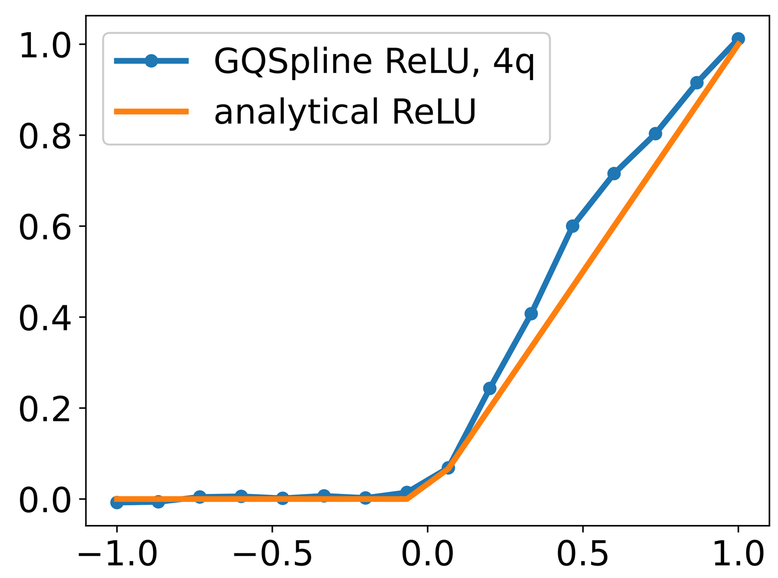
Motivation

- Physical phenomena are often modeled as partial differential equations. Applications: electromagnetics, fluid dynamics, heat conduction, mechanics etc.
- Besides traditional numerical methods used to solve PDEs, an emerging strategy in QML, is to use a parameterized quantum circuit as a physics informed neural network **(QPINN)**.
- Except that classical layers are used in literature for nonlinear activation functions.
  $\implies$ hybrid classical/quantum PINNs
- **Objective:** Combine a QPINN, with an ansatz pre-trained to compute nonlinear activation functions.
- **How?** Represent activation function with a B-spline, use a variational quantum linear solver to compute coefficients. Query trained ansatz in QPINN training.

Hybrid QPINNs



Q-Splines for Activation Functions



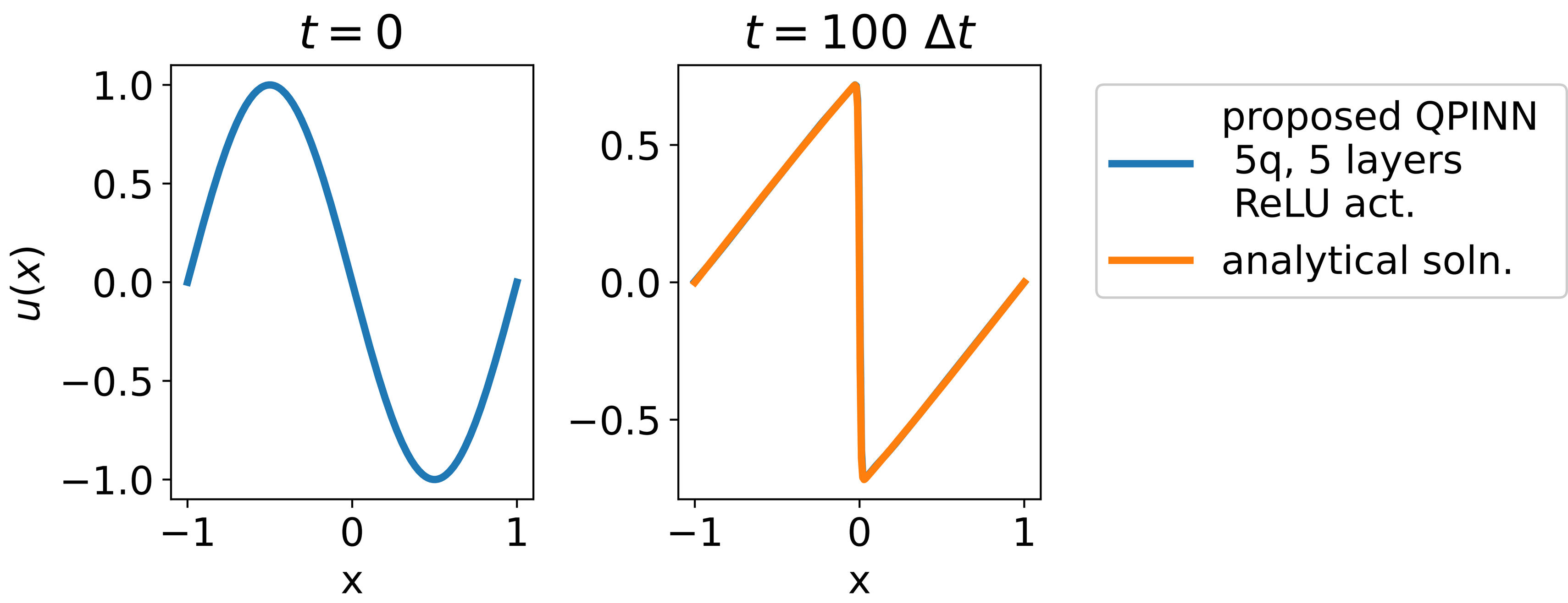
Activation functions approximated as piecewise linear B-splines [2].

$$\mathbf{actf}_i = S * \mathbf{coeff}_i$$

S : matrix of basis expansions
$\mathbf{actf}_i$: activation func. evaluations

- $\mathbf{coeff}_i = VQLS(S, \mathbf{act}_i)$
- Output optimal weights of trained ansatz.

1D Burger's eqn.



Governing eqn. $u_t + uu_x = \frac{0.01}{\pi} u_{xx}$

initial cond. $u(x, 0) = -\sin(\pi x)$

boundary cond. $u(-1, t) = u(1, t) = 0$

- **Losses** Physics loss: 10,000 collocation points.
  BC/IC loss: 50 points for initial data, 25 each at boundaries.
- **Training** Adam optimizer, 2000 epochs.
- **Compare** Hybrid QPINN [1] v. QSpline activated QPINN.
  46% fewer tunable params required for similar accuracy.

References

1. Trahan C, Loveland M, Dent S. **Quantum Physics-Informed Neural Networks**. *Entropy*. 2024; 26(8):649. `https://doi.org/10.3390/e26080649`
2. Inajetovic, M.A., Orazi, F., Macaluso, A., Lodi, S., Sartori, C. **Enabling Non-linear Quantum Operations Through Variational Quantum Splines**. ICCS 2023. `https://doi.org/10.1007/978-3-031-36030-5_14`