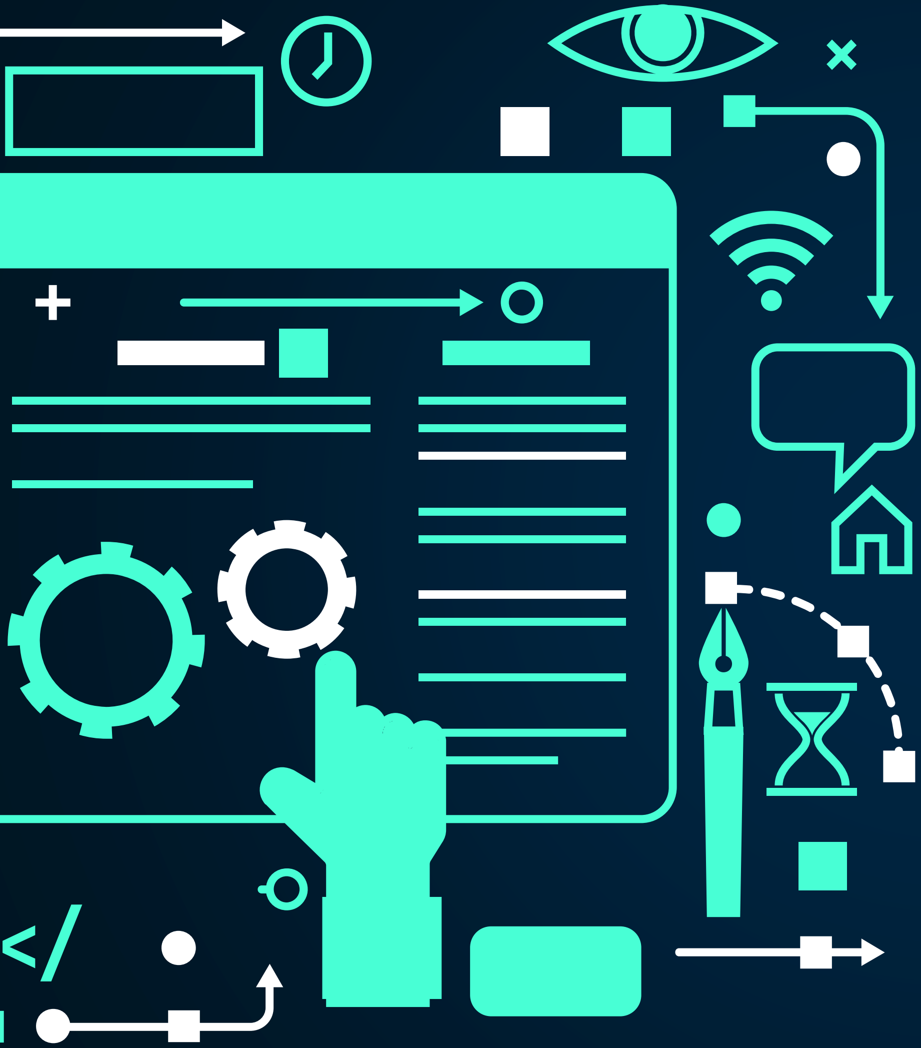

Physics @ UFABC

JC: SOLVING NONLINEAR DIFERENTIAL EQUATIONS WITH DIFERENTIABLE QUANTUM CIRCUITS

Carolina Perdomo

References:

[arxiv.org/abs/2011.10395]

MAIN POINTS

Solving nonlinear differential equations with differentiable quantum circuits

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(Dated: May 20, 2021)

We propose a quantum algorithm to solve systems of nonlinear differential equations. Using a quantum feature map encoding, we define functions as expectation values of parametrized quantum circuits. We use automatic differentiation to represent function derivatives in an analytical form as differentiable quantum circuits (DQCs), thus avoiding inaccurate finite difference procedures for calculating gradients. We describe a hybrid quantum-classical workflow where DQCs are trained to satisfy differential equations and specified boundary conditions. As a particular example setting, we show how this approach can implement a spectral method for solving differential equations in a high-dimensional feature space. From a technical perspective, we design a Chebyshev quantum feature map that offers a powerful basis set of fitting polynomials and possesses rich expressivity. We simulate the algorithm to solve an instance of Navier-Stokes equations, and compute density, temperature and velocity profiles for the fluid flow in a convergent-divergent nozzle.

- HYBRID QUANTUM-CLASSICAL WORKFLOW
- DQC[1]S ARE TRAINED TO SATISFY DIFERENTIAL EQUATIONS
- DIFFERENT EXAMPLES TO SHOW ALGORITHM ADAPTABILITY

[1] **DQC**: Differential Quantum Circuit [arxiv.org/abs/2011.10395]

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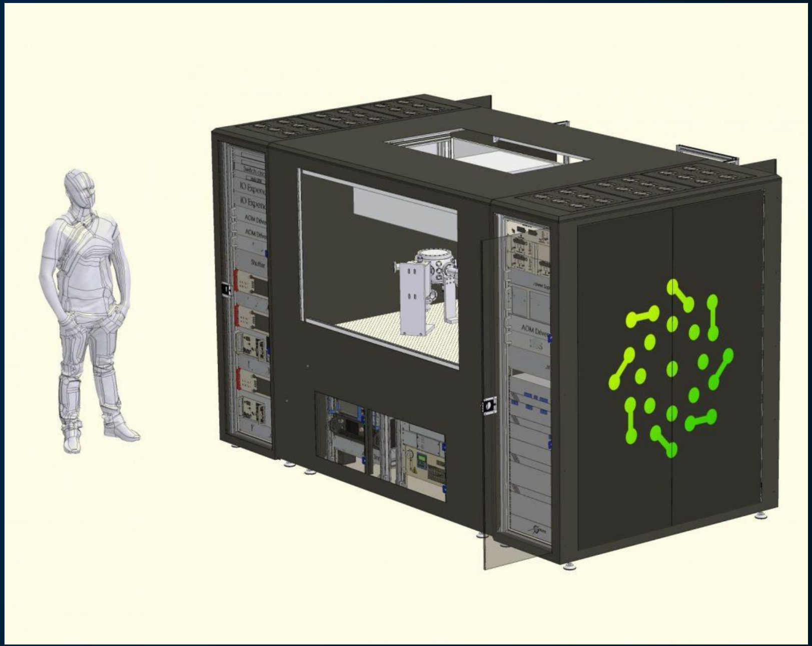


01. INTRODUCTION

- Era of the first available quantum computers.
- Although still imperfect: Noisy Intermediate-Scale Quantum devices (NISQ).
- Hybrid Quantum/Classical computation.

Boosting advancements in quantum chemistry

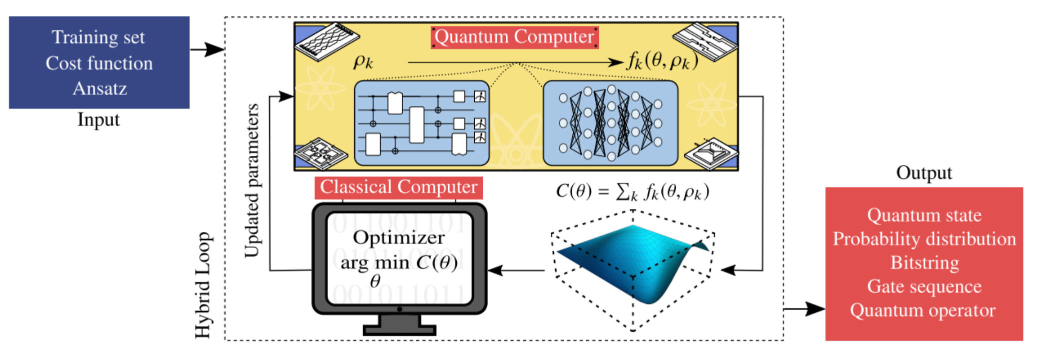
Pasqal and Rahko will jointly develop algorithms to solve advanced chemistry problems, and fully implement them on Pasqal's upcoming

Accelerating High-Performance Computing

Through a collaboration with Atos, the global leader in digital transformation, Pasqal is striving to incorporate its quantum processors into high-performance computing environments, thereby setting the stage for an era of hybrid quantum-HPC systems with potential for short-term, real-world applications.

TECHNICAL CONTEXT

VARIATIONAL QUANTUM ALGORITHMS



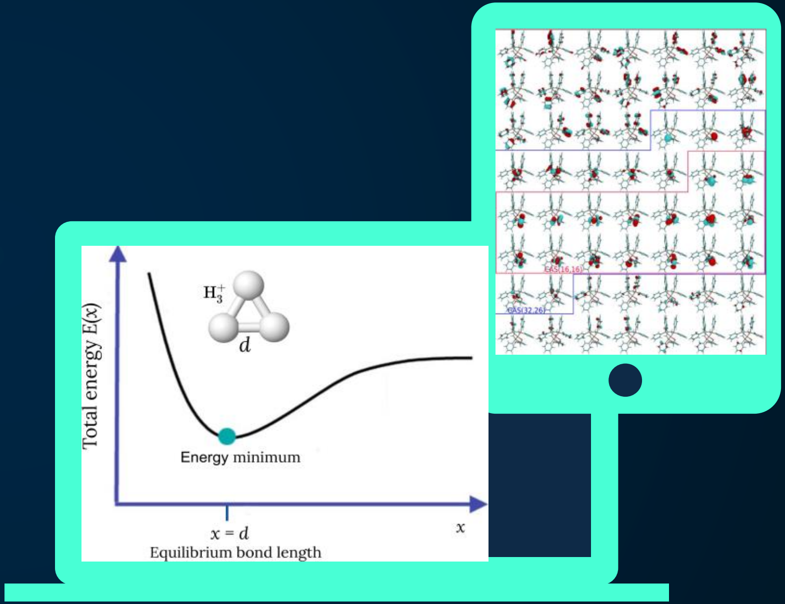
VARIATIONAL QUANTUM SOLVERS

Use a variational quantum algorithm for solving DEs.

POTENTIAL USE –CASES OF VQA

CHEMICAL ENGINEERING

CLIMATE[2]

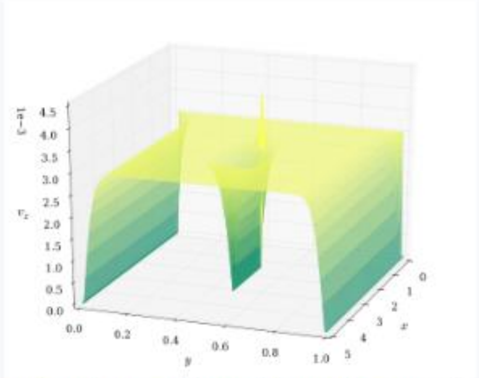


[2] Quantum computing enhanced computational catalysis arXiv:2007.14460

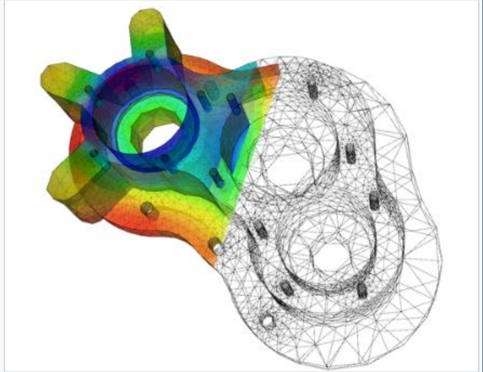
WHY WE WANT TO STUDY DE?

Many industrial models can be model with DE.
Why? In essence, DE describes some rate of changes or some conservation law. So, they're describing physics or rules about the system.

PHYSICS SIMULATIONS



Navier–Stokes differential equations used to simulate airflow around an obstruction


Visualization of heat transfer in a pump casing, created by solving the heat equation. Heat is being generated internally in

PROCESSES GOVERNED BY DIFFERENTIAL EQUATIONS

Heat transfert, fluid or air flows, stress and strain, chemical reactions, etc

QUANTUM COMPUTATION AND DIFFERENTIAL EQUATIONS

Finding solutions to nonlinear systems of DEs is challenging.

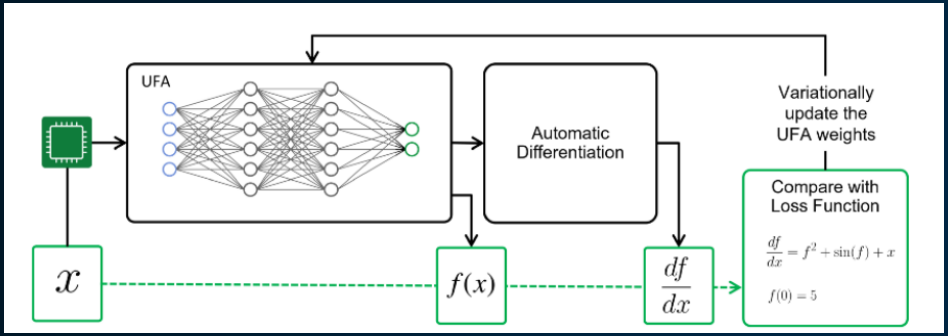
Quantum computers offer a fundamentally different approach to perform computation.

Finding NISQ protocols that can offer advantage for industrially relevant tasks represents an open challenge.

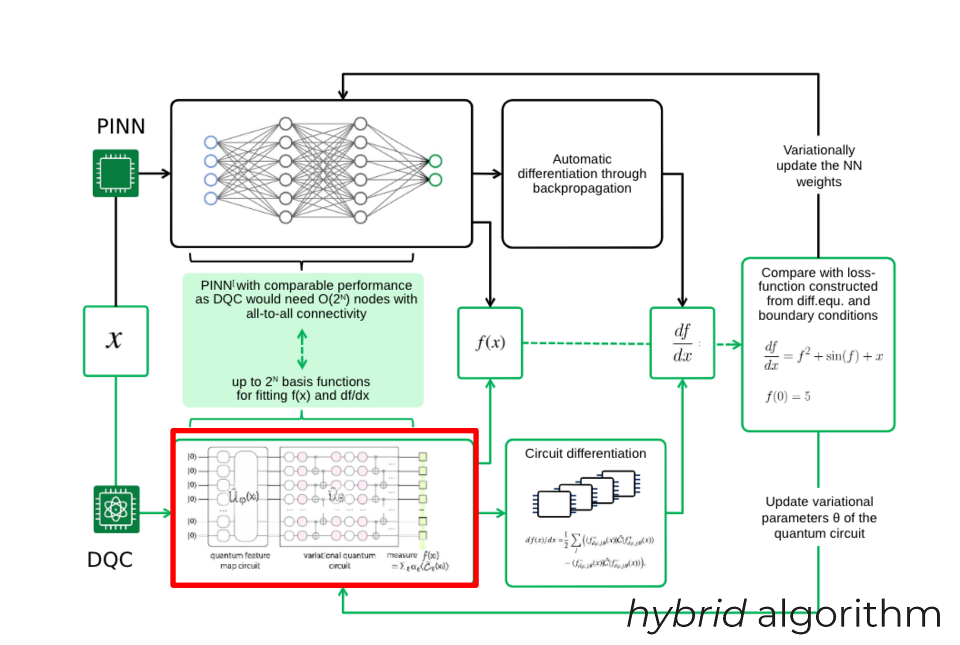
- Many industry-relevant problems can be modelled by differential equations.
- These equations are typically very challenging to solve with classical computers.

—SUMMARY

02. DQC ALGORITHM



- Classical neural networks are considered among the most promising directions.



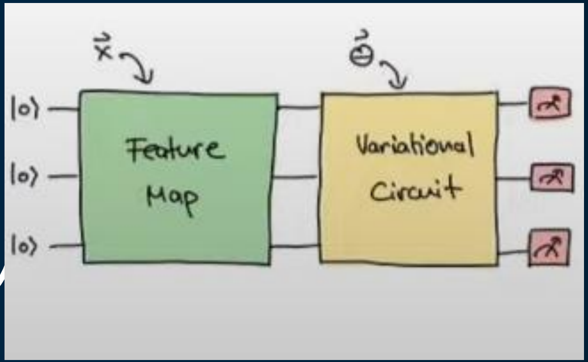
WHAT CAN WE LEARN FROM THE CLASSICAL NEURAL NETWORKS APPROACH?

03. IMPLEMENTATIONS STEPS

FEATURE MAP
Encoder

Differential equation

VQC
Represents functions derivatives analytically.

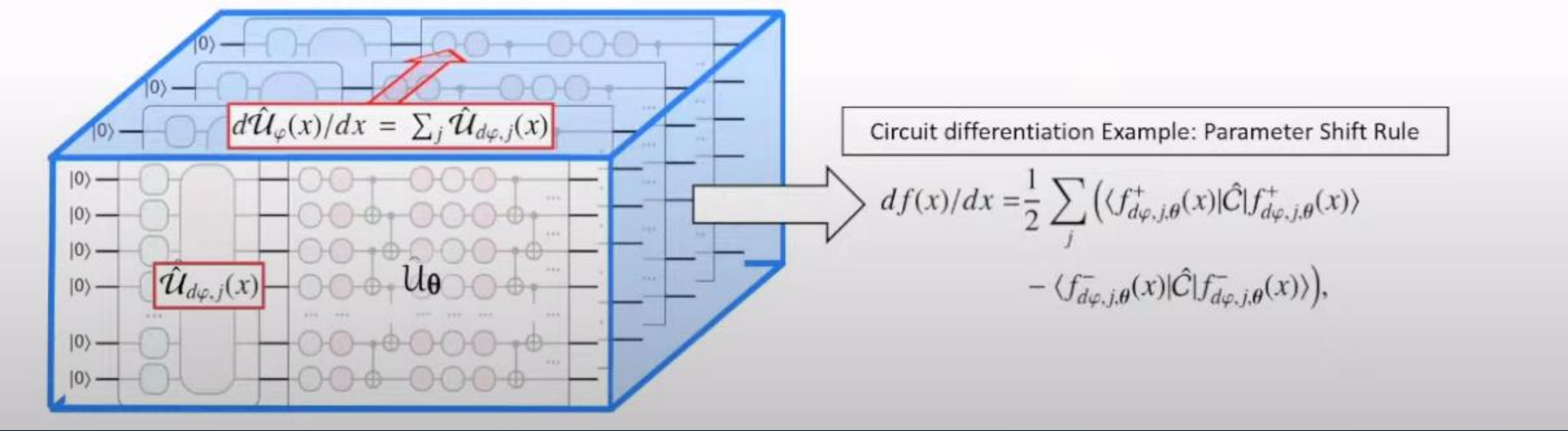


$$f(x) = \langle f_{\varphi,\theta}(x)\boxed{|\hat{C}|}f_{\varphi,\theta}(x)\rangle$$

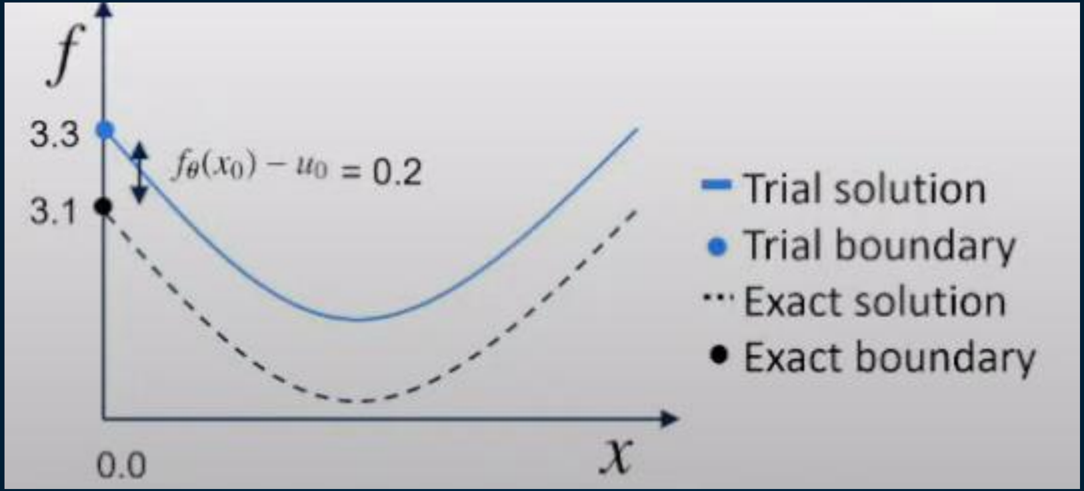
Uniquely maps distinct wavefunctions to distinct expectation values.

After: How can we compute the derivatives?

The parameter-shift rule gives the correct gradient
up to the available numerical precision.

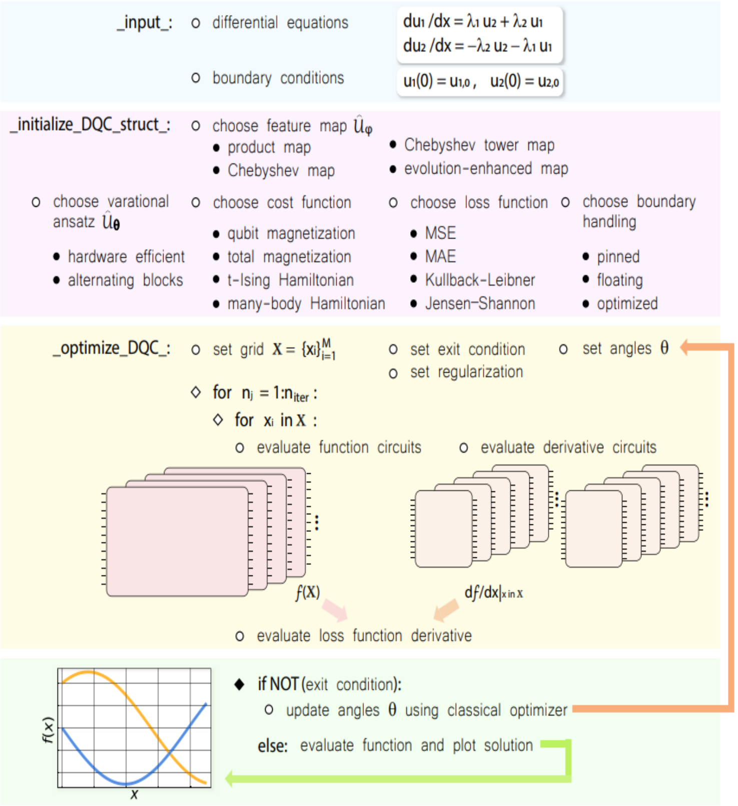


Loss function:



We want to quantify how good the trial solution "solves" the DE.

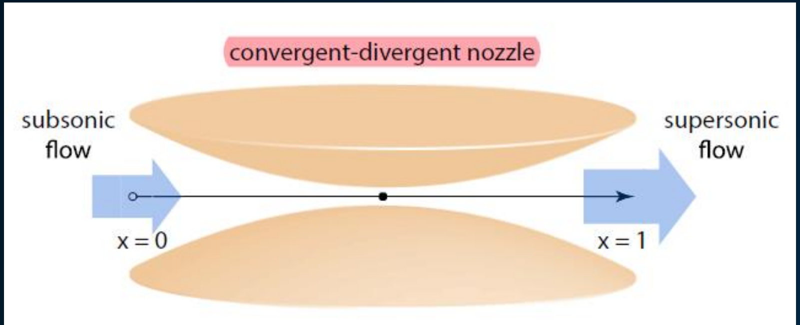
$$\mathcal{L}_{\boldsymbol{\theta}}[d_x f, f, x] = \mathcal{L}_{\boldsymbol{\theta}}^{(\mathrm{diff})}[d_x f, f, x] + \mathcal{L}_{\boldsymbol{\theta}}^{(\mathrm{boundary})}[f, x]$$



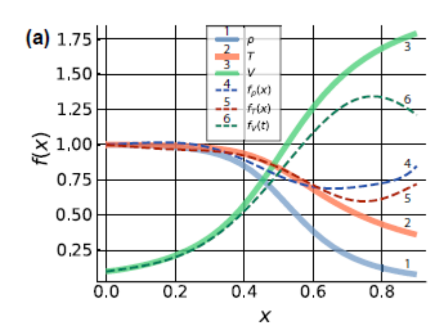
Basically:

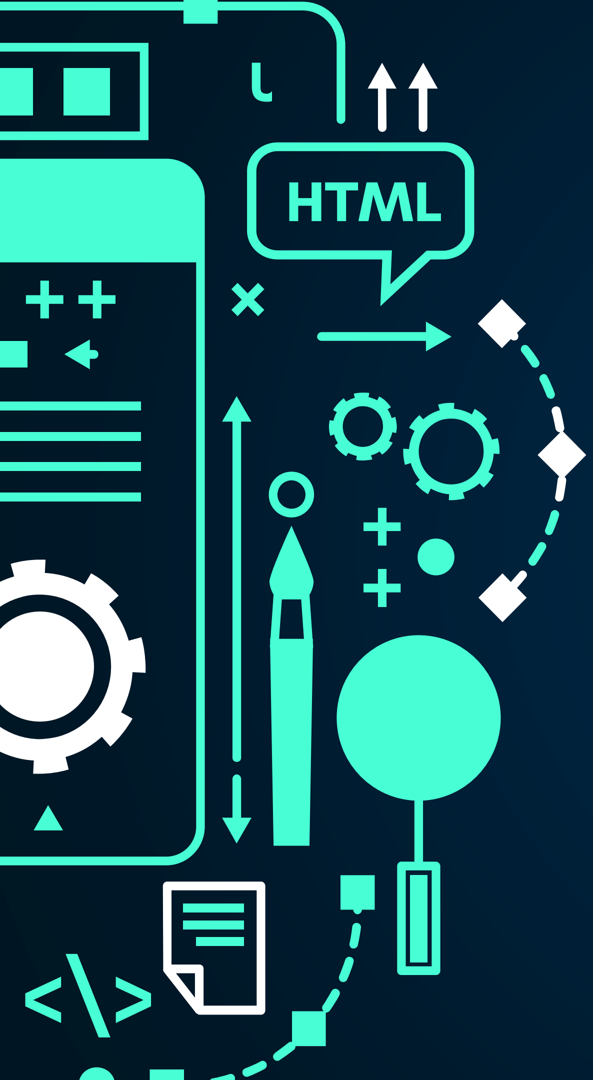
You can have several versions of the same algorithm depending on what you choose!

USE-CASE EXAMPLE IN THE REAL-WORLD: FLUID DYNAMICS



$$\frac{\partial \rho}{\partial t} = -\rho\frac{\partial V}{\partial x} - \rho V\frac{\partial(\ln A)}{\partial x} - V\frac{\partial \rho}{\partial x},$$
$$\frac{\partial T}{\partial t} = -V\frac{\partial T}{\partial x} - (\gamma - 1)T\left(\frac{\partial V}{\partial x} + V\frac{\partial(\ln A)}{\partial x}\right),$$
$$\frac{\partial V}{\partial t} = -V\frac{\partial V}{\partial x} - \frac{1}{\gamma}\left(\frac{\partial T}{\partial x} + \frac{T}{\rho}\frac{\partial \rho}{\partial x}\right),$$





THANKS!
Any question?