An Introduction to the Synergy of Deep Learning and Differential Equations

Seminar

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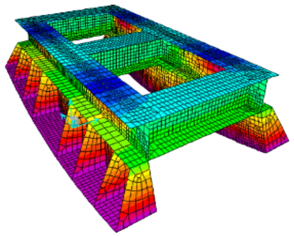
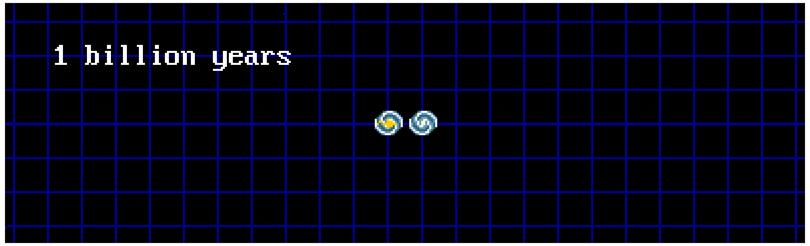
Motivation

- Differential equations are the **language of nature**
- Prominent role in many disciplines including engineering, physics, economics, and biology

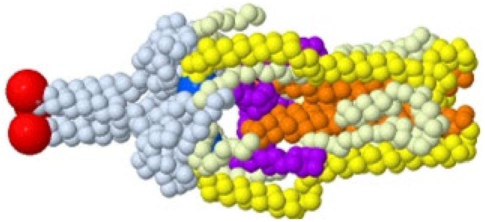


Engineering: Structural analysis with finite element method



Physics: universe expansion

Finance: Black Scholes pricing model



Biology: Spike protein transformation in Covid-19

What is a Differential Equation?

- A function that takes as input the spatial or **spatio-temporal coordinates x** and, optionally, derivatives of the **unknown Φ** with respect to these coordinates

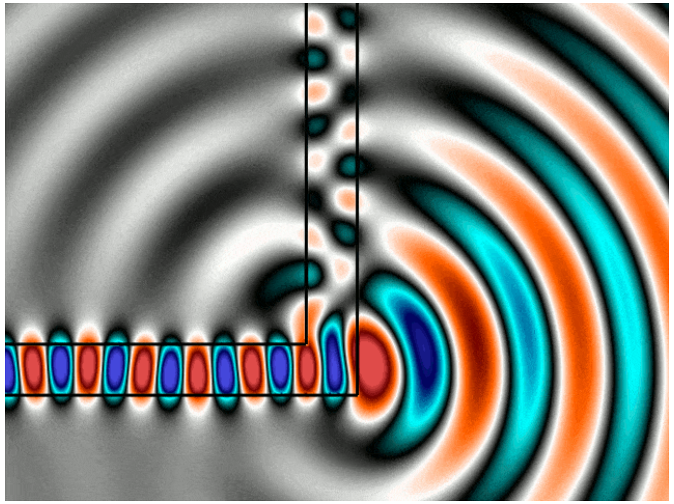
$$F\left(\mathbf{x}, \Phi, \nabla_{\mathbf{x}}\Phi, \nabla^2_{\mathbf{x}}\Phi, \ldots\right) = 0, \quad \Phi : \mathbf{x} \mapsto \Phi(\mathbf{x}).$$

Implicit Formulation of a Differential Equation

- An example from physics

$$\frac{\partial \Phi}{\partial t} - c^2 \frac{\partial \Phi}{\partial \mathbf{x}} = 0.$$

Helmoltz Wave Equation



A More Familiar Example

- Second Newton's law:

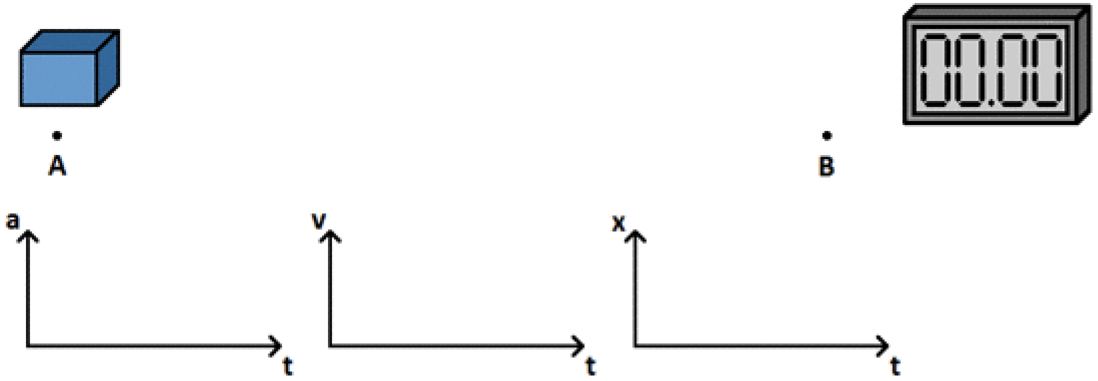
$$F = ma$$

- *Acceleration is the second derivative of the position!*
- So this becomes:

$$F = m\frac{d^2x(t)}{dt^2}$$

In the *implicit (equation=0)* form:

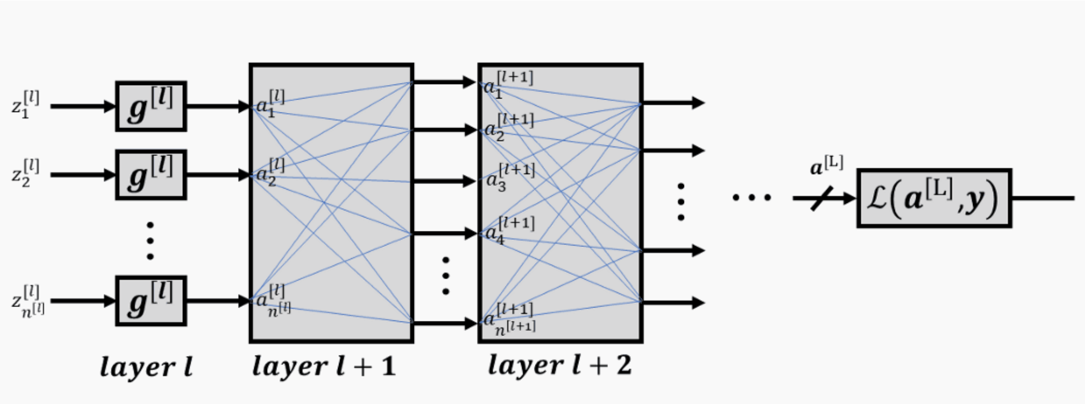
$$F - m\frac{d^2x(t)}{dt^2} = 0$$



Massive object subject to a force

Backpropagation

- Deep Learning is deeply intertwined with Differential Equations with the **backpropagation**

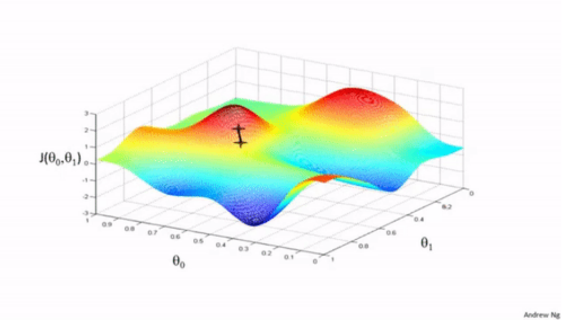


$$\frac{\partial \mathcal{L}}{\partial z^{[l-1]}} = \left[W^{[l]}\right]^{\mathrm{T}} \cdot \frac{\partial \mathcal{L}}{\partial z^{[l]}} * g^{[l-1]\prime}\left(z^{[l-1]}\right)$$

$$\frac{\partial \mathcal{L}}{\partial W^{[l]}} = \frac{\partial \mathcal{L}}{\partial z^{[l]}} \cdot \left[a^{[l-1]}\right]^{\mathrm{T}}$$

$$\frac{\partial \mathcal{L}}{\partial b^{[l]}} = \frac{\partial \mathcal{L}}{\partial z^{[l]}}$$

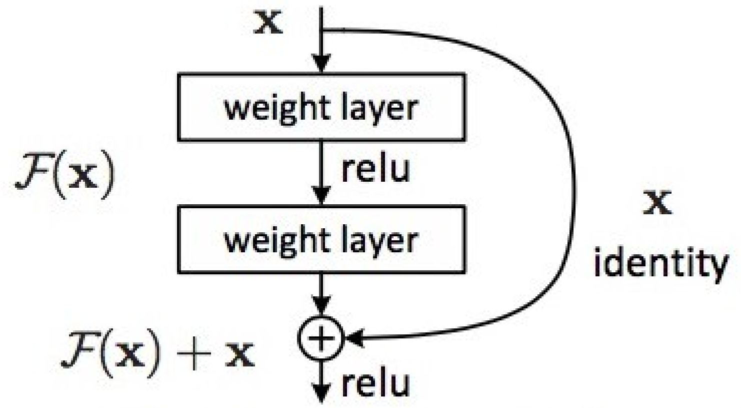
- ➢ We use information of the **gradients** to update a network parameters!



Gradient descent in 2 dimensions

Neural Ordinary Differential Equations

- ResNet [1] have *skip connections* between layers



Residual connection

$$x_{k+1} = F(x_k) + x_k$$

This resembles

$$\frac{x_{k+1} - x_k}{\Delta t} = F(x_k) \approx \frac{dx}{dt} \; for \; \Delta t = 1$$

- ➢ We can build Neural Ordinary Differential Equations [2](Neural ODEs)!
- ➢ Networks tied to numerical solver with inference model:

$$x_T = x_0 + \int_0^T \boldsymbol{F_\theta}\big(t, x(t)\big)dt$$

[1] Kaiming, et al. Deep residual learning for image recognition. In: Proceedings of the IEEE conference on computer vision and pattern recognition. 2016. p. 770-778.
[2] CHEN, Ricky TQ, et al. Neural ordinary differential equations. NeurIPS 2018

Neural Ordinary Differential Equations

- Networks tied to numerical solver with inference model:

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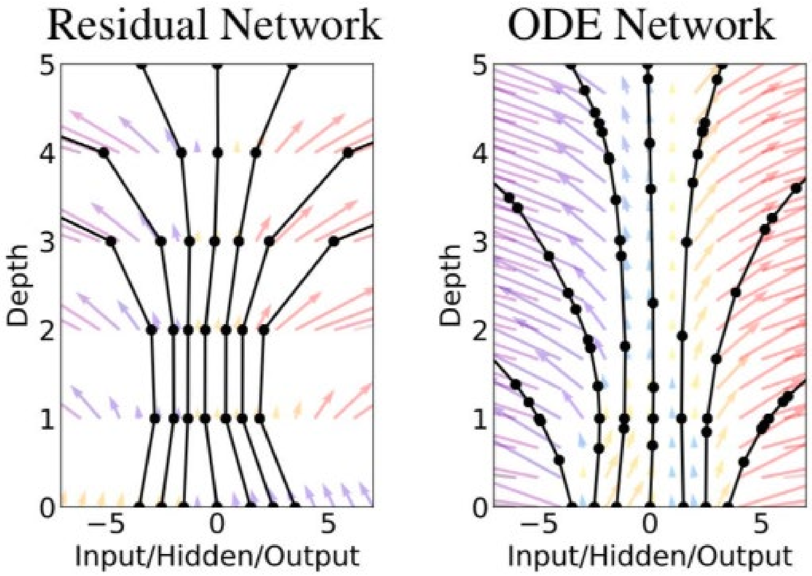
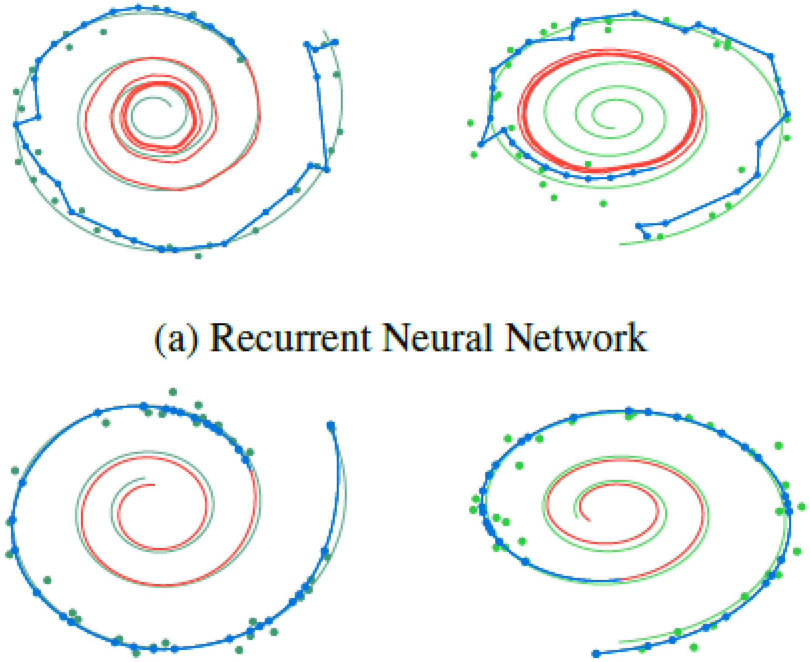


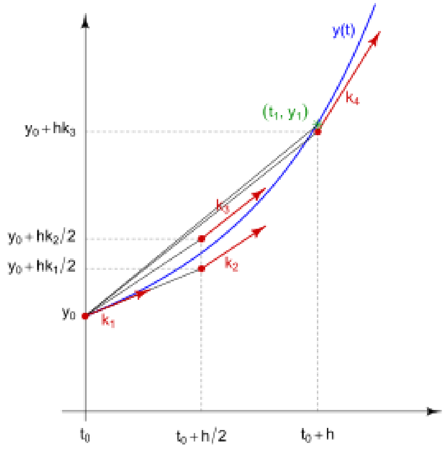


(a) Recurrent Neural Network

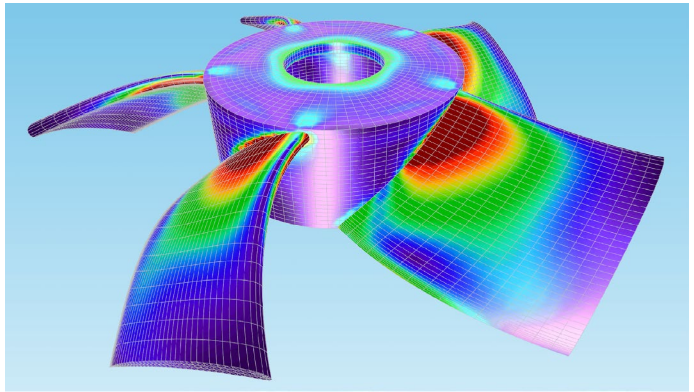
(b) Latent Neural Ordinary Differential Equation

Physics Simulation

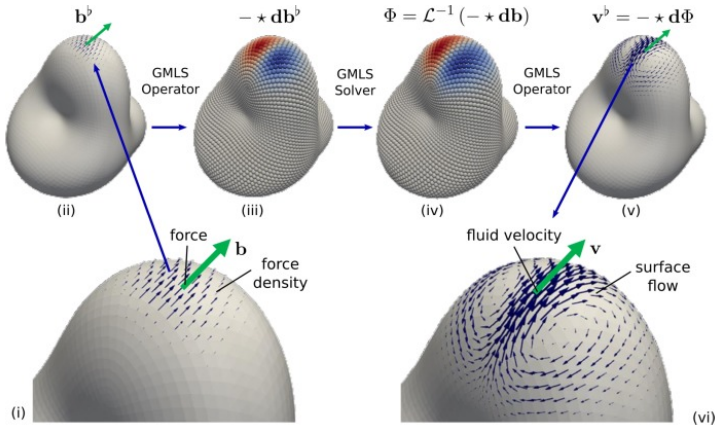
- Classical approaches can be extremely slow or even fail to represent complex behaviors
- Need to choose the right step sizes
- If adaptive solvers are used, it may take too long to solve and simulate a physics process
- Also, **discretizations** are inherently "wrong" → physics are mostly **continuous**!



Runge-Kutta method for ODEs



Finite Element Method (FEM)



Mesh-free methods (e.g. particle)

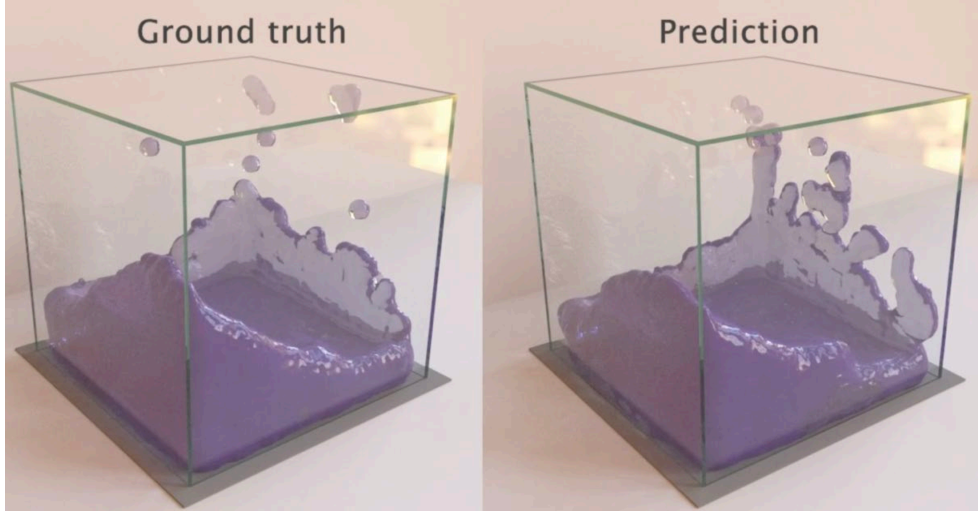
Learning Simulations

Engineered simulators

- Substantial effort to build
- Substantial resources to run
- Only as accurate as the model
- Not always suitable for solving inverse problems

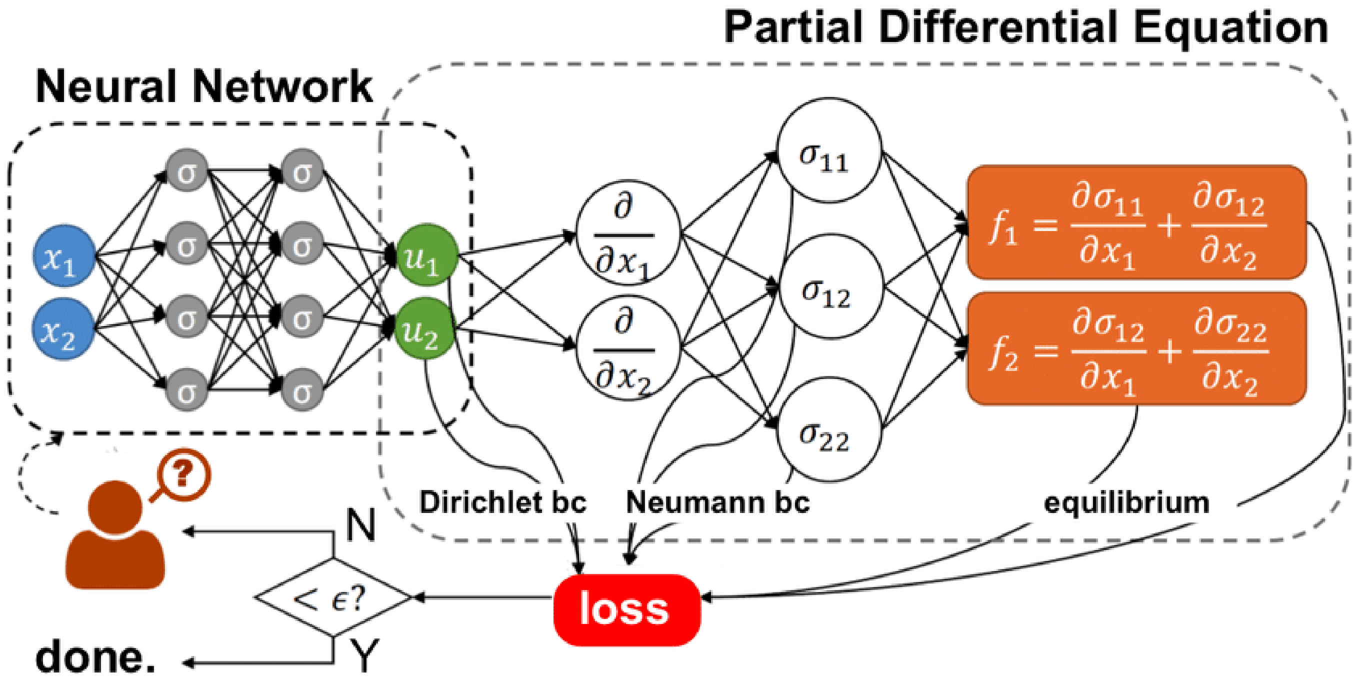
Learned simulators

- Reusable general architectures
- Can be directly optimized for efficiency
- Can be as accurate as the available data
- Gradient-based search for control, inference, etc



Physics Informed Neural Networks

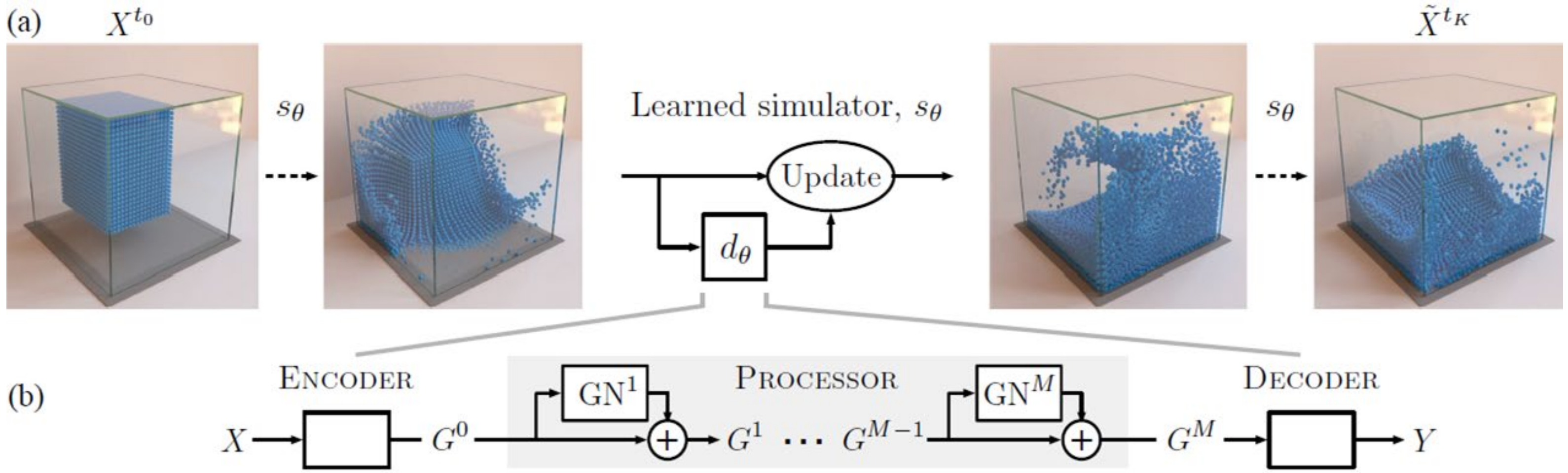
- What if we use Deep Learning to solve Differential Equations?
- ➢ PINNs: Physics Informed Neural Networks[1]



[1] RAISSI, Maziar; PERDIKARIS, Paris; KARNIADAKIS, George E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 2019, 378: 686-707.

Graph Networks Simulators

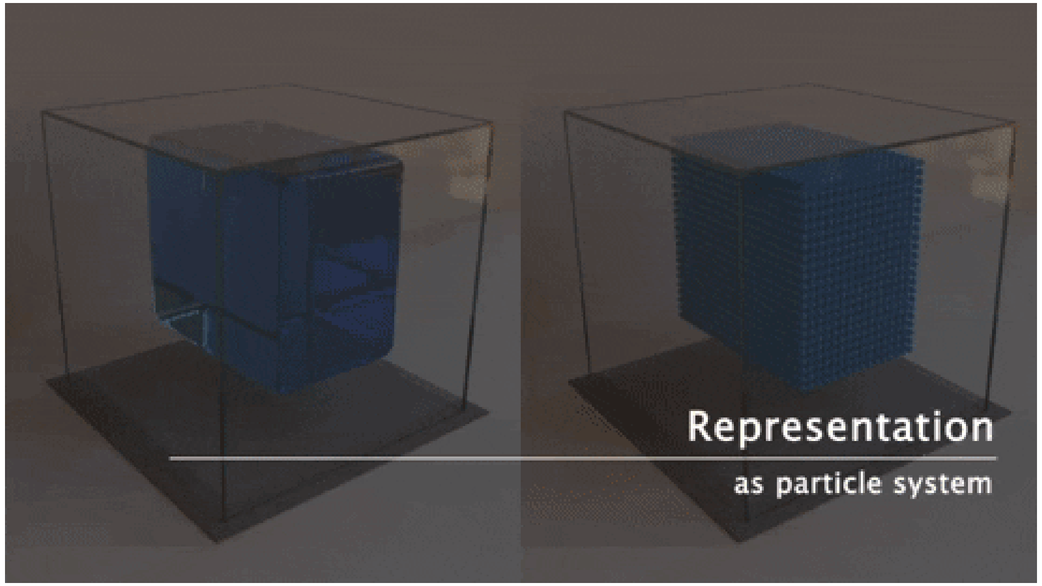
- Many problems can can be discretized in **particles** or **mesh points**
- What If we use Graphs Networks to model these interactions?
- ➢ GNS: Graph-based Neural Simulators [1]
- ➢ A graph of neighboring particles is created ar

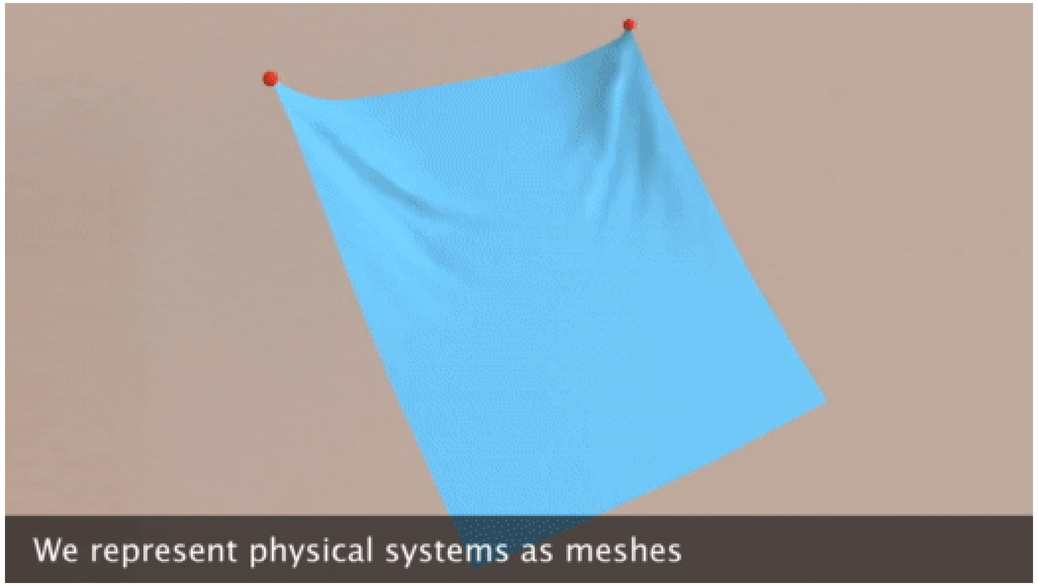


[1] Sanchez-Gonzalez, Alvaro, et al. "Learning to simulate complex physics with graph networks." *International Conference on Machine Learning*. PMLR, 2020

Graph Networks Simulators

- GNS: Graph-based Neural Simulators [1]
- We can also expand to mesh-based models [2]





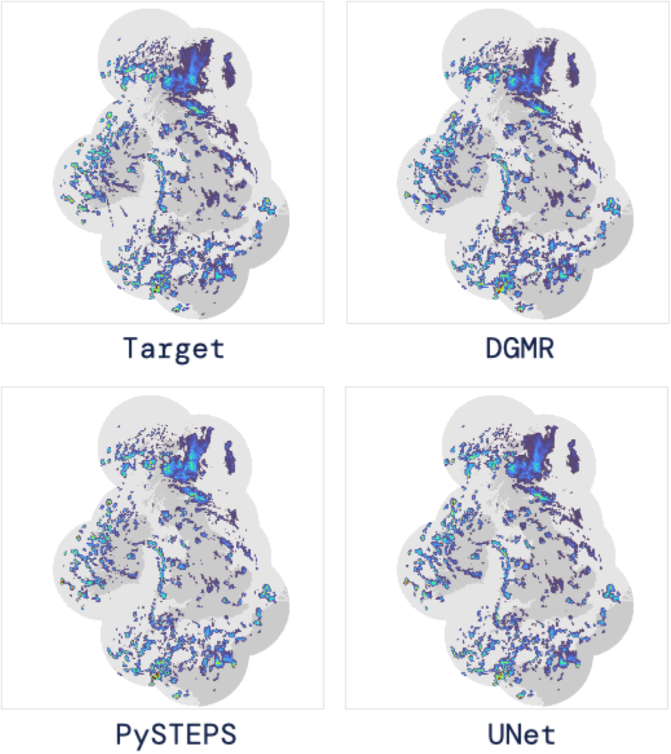
[1] Sanchez-Gonzalez, Alvaro, et al. "Learning to simulate complex physics with graph networks." *International Conference on Machine Learning*. PMLR, 2020
[2] Pfaff, Tobias, et al. "Learning mesh-based simulation with graph networks." *International Conference on Learning Representations.* ICLR, 2021

Latest Advances: Blazing Fast Weather Simulation

- Deepmind has created a weather model which is thousand of times faster than numerical simulations [1]
- Yet, it can forecast weather almost perfectly!

$$P(\mathrm{X}_{M+1:M+N} \mid \mathrm{X}_{1:M}) \\ = \int P(\mathrm{X}_{M+1:M+N} \mid \mathrm{Z}, \mathrm{X}_{1:M}, \theta) P(\mathrm{Z} \mid \mathrm{X}_{1:M}) d\mathrm{Z}.$$

Radar model in differential form



[1] RAVURI, Suman, et al. Skillful Precipitation Nowcasting using Deep Generative Models of Radar. arXiv preprint arXiv:2104.00954, 2021.

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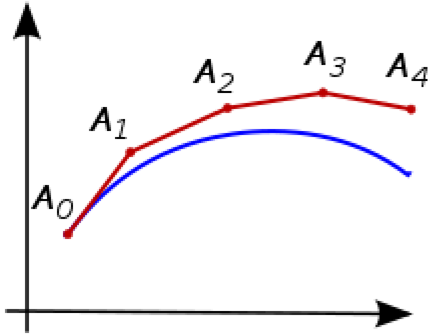
Hypersolvers: Best of Both Worlds?

- When solving Differential Equations numerically, we need to take **integration steps**
- For each integration step, we have a **discretization error**



- **Hypersolvers:** we can learn to **correct this error** [1]

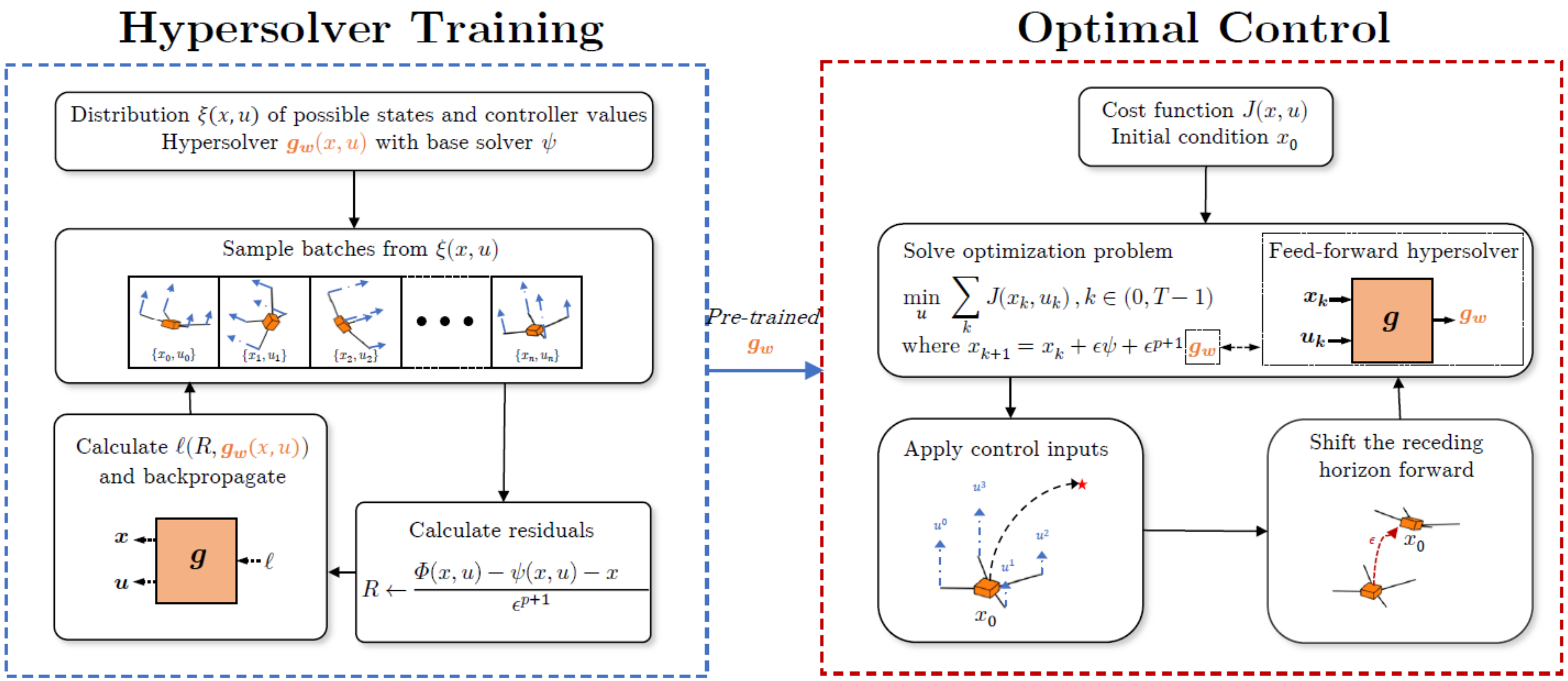
$$x_{k+1} = x_k + \underbrace{\epsilon \psi_\epsilon (t_k, x_k, u_k)}_{\text{base solver step}} + \boxed{\epsilon^{p+1} \underbrace{g_\omega (t_k, x_k, u_k)}_{\text{approximator}}}$$

- The error has *theoretical bounds,* which is very important in practice

[1] Poli M, Massaroli S, Yamashita A, Asama H, Park J. Hypersolvers: Toward fast continuous-depth models. NeurIPS 2020

Hypersolvers: an Application to Control

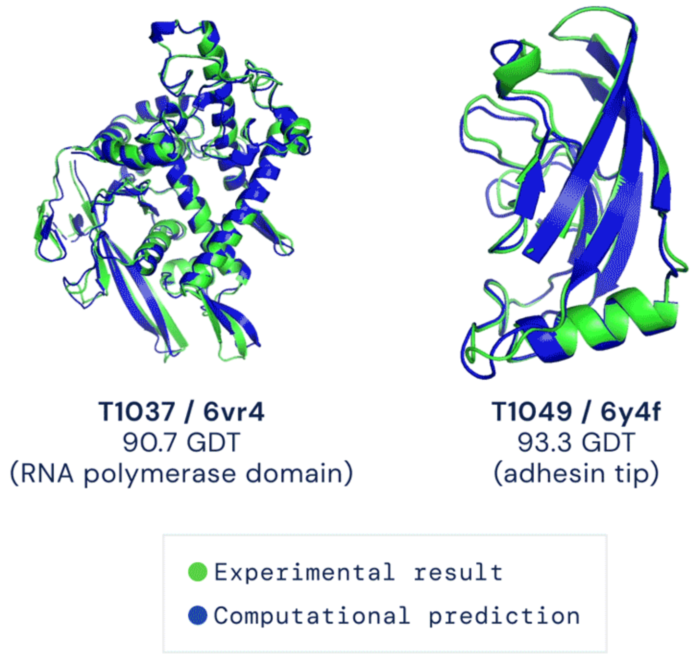
- We can apply the idea to **speed up** optimal control! [1]



[1] Berto, Federico, et al. Neural Solvers for Fast and Accurate Numerical Optimal Control. NeurIPS DLDE Workshop, 2021

Conclusion

- Differential equations describe the reality around us
- Differential Equations and Deep Learning are deeply intertwined
- We can use Deep Learning to simulate and learn the world we live in!



A Final Quote

"Differential equations won't help you much in the design of airplanes — not yet, anyhow."

Nevil Shute, British Aeronautical Engineer, 1923

After a 100 years, the time has come to design airplanes and so much more!

DAEWOONG

Thanks for your attention

Do not hesitate to contact us for any doubts or ideas!

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