Reducing the computational cost of solving ODE systems via machine learning

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Reducing the complexity of chemical networks via interpretable autoencoders

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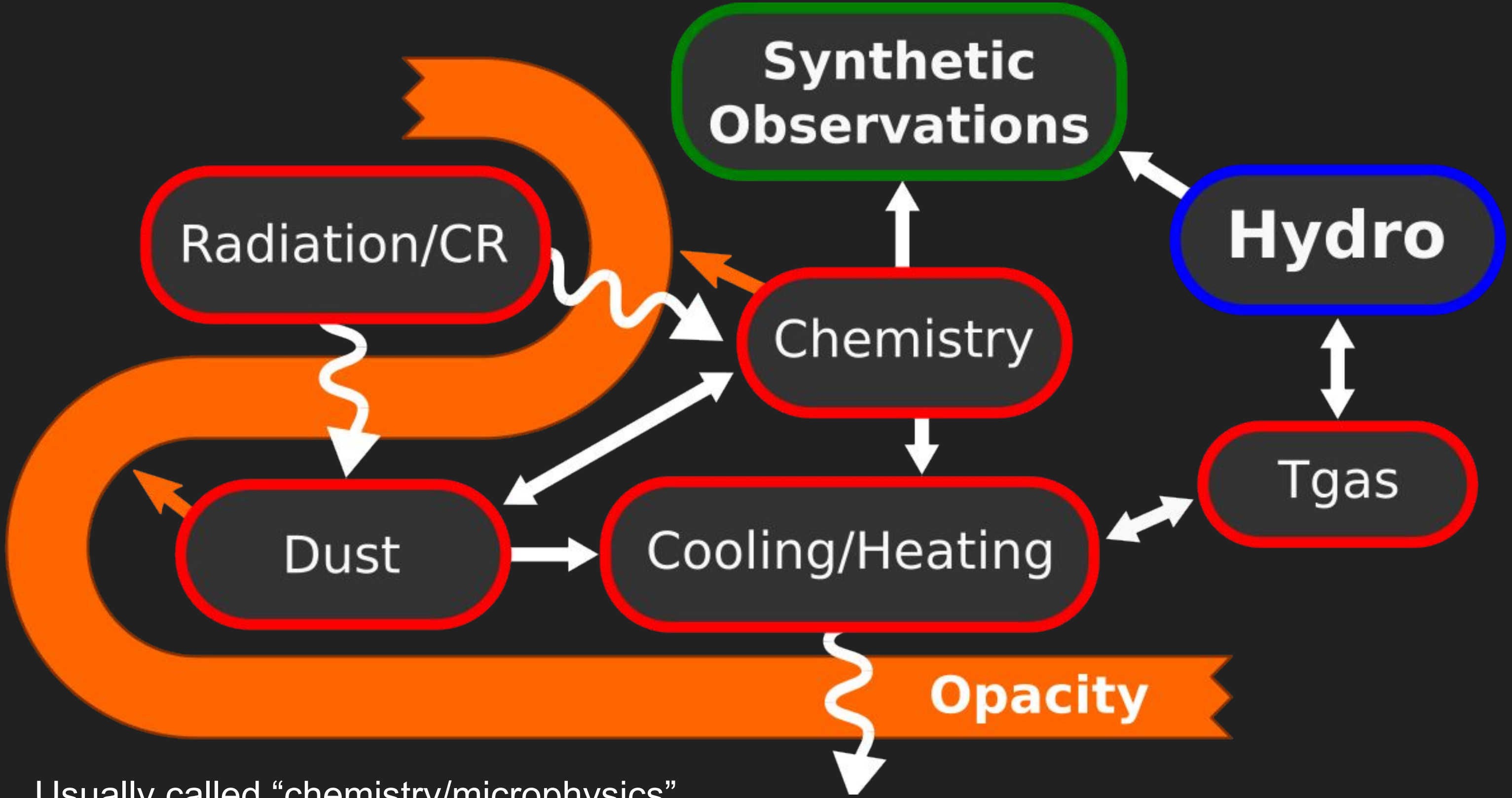
Outline

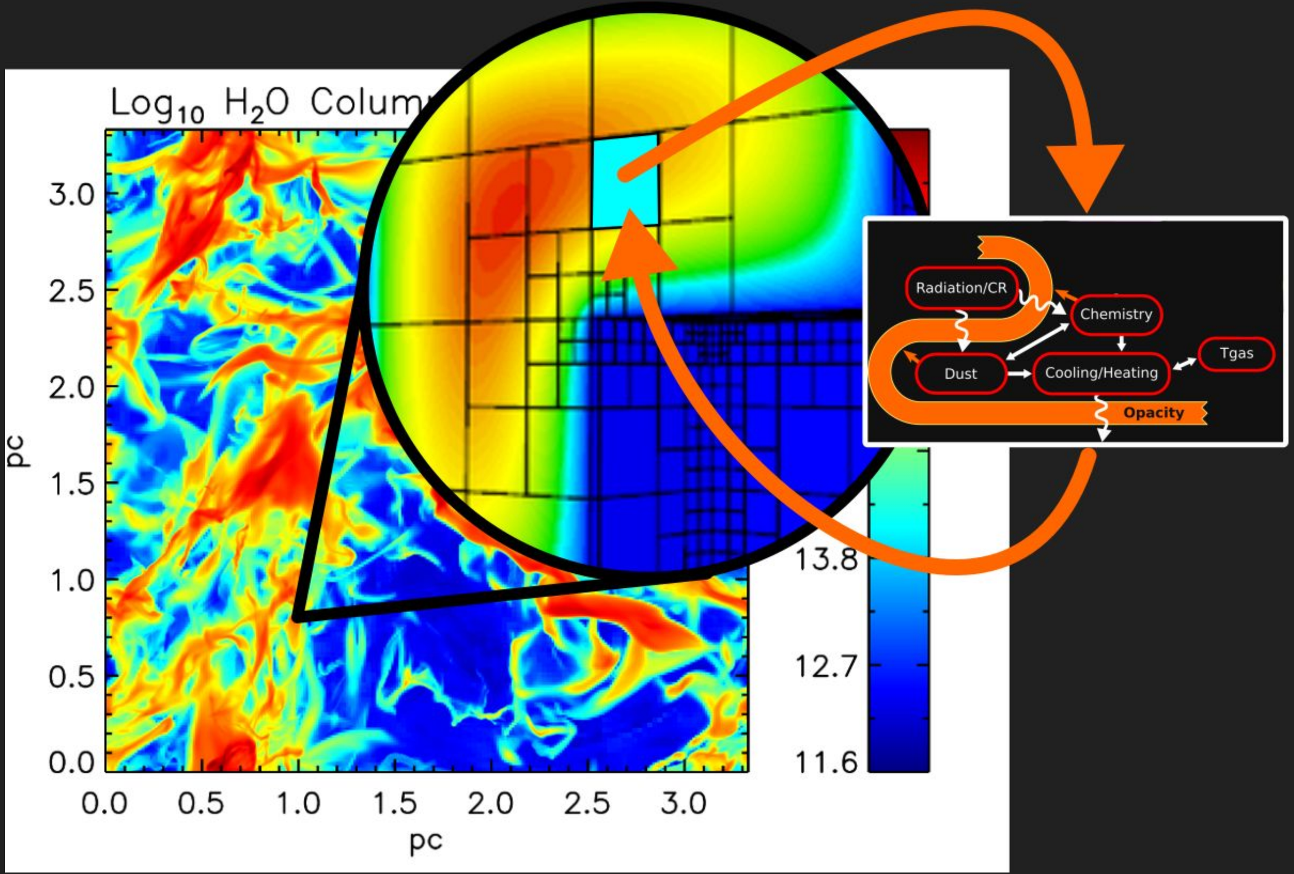
1. Astrophysical Context
2. System of Ordinary Differential Equations (ODEs)
3. ODE systems in (astro)chemistry
4. Deep Neural Networks (DNNs)
5. DNN Autoencoders
6. Our Method: ODEs + Autoencoders

Context /1



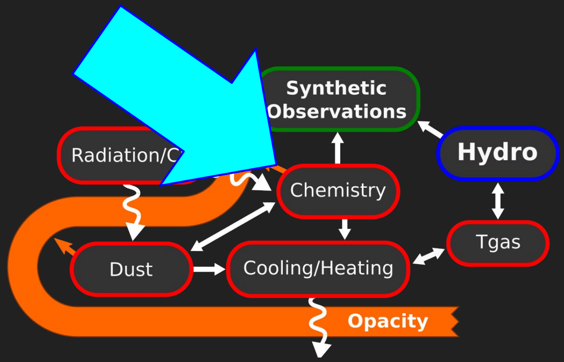
Usually called “chemistry/microphysics”

Context /2



Computational Overhead

Chemistry



$$\boxed{\mathrm{C} + \mathrm{O}} \leftrightharpoons \boxed{\mathrm{CO}}$$

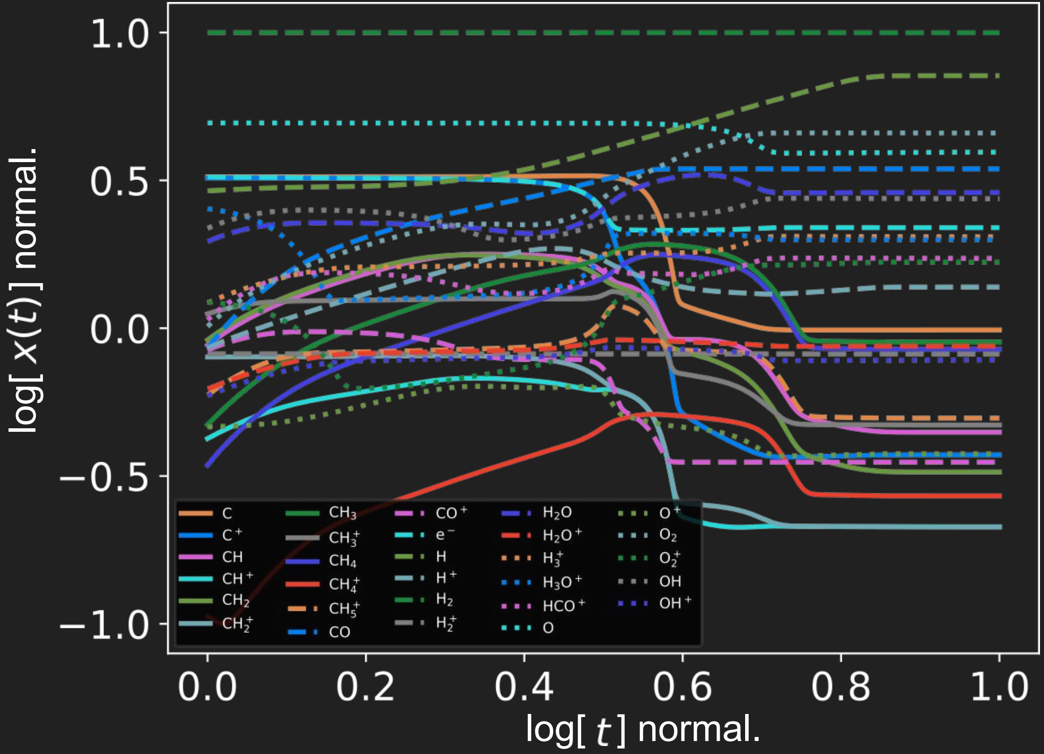
$$\frac{\mathrm{d}x_{\mathrm{C}}}{\mathrm{d}t} = \frac{\mathrm{d}x_{\mathrm{O}}}{\mathrm{d}t} = -\boxed{k_1\, x_{\mathrm{C}}\, x_{\mathrm{O}}} + \boxed{k_2\, x_{\mathrm{CO}}}$$

$$\frac{\mathrm{d}x_{\mathrm{CO}}}{\mathrm{d}t} = +\boxed{k_1\, x_{\mathrm{C}}\, x_{\mathrm{O}}} - \boxed{k_2\, x_{\mathrm{CO}}}$$

$$\dot{\bar{x}} = f(\bar{x}; k)$$

Solving ODEs

Advance x(t) in time with BDF solving $\dot{x} = f(\bar{x}; k)$



Typical networks

Species → Reactions

Primordial: 10 → 30

MC (hydro): 40 → 300

MC (0D): 450 → 4500+

Disk: 450+ → 5000+

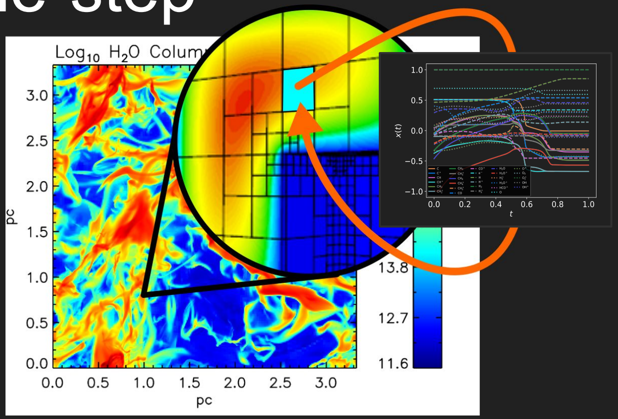
This Example: 29 → 224

PROBLEM

Integrating for a (hydro) time-step

$$\dot{x} = f(\bar{x}; k)$$

for each cell



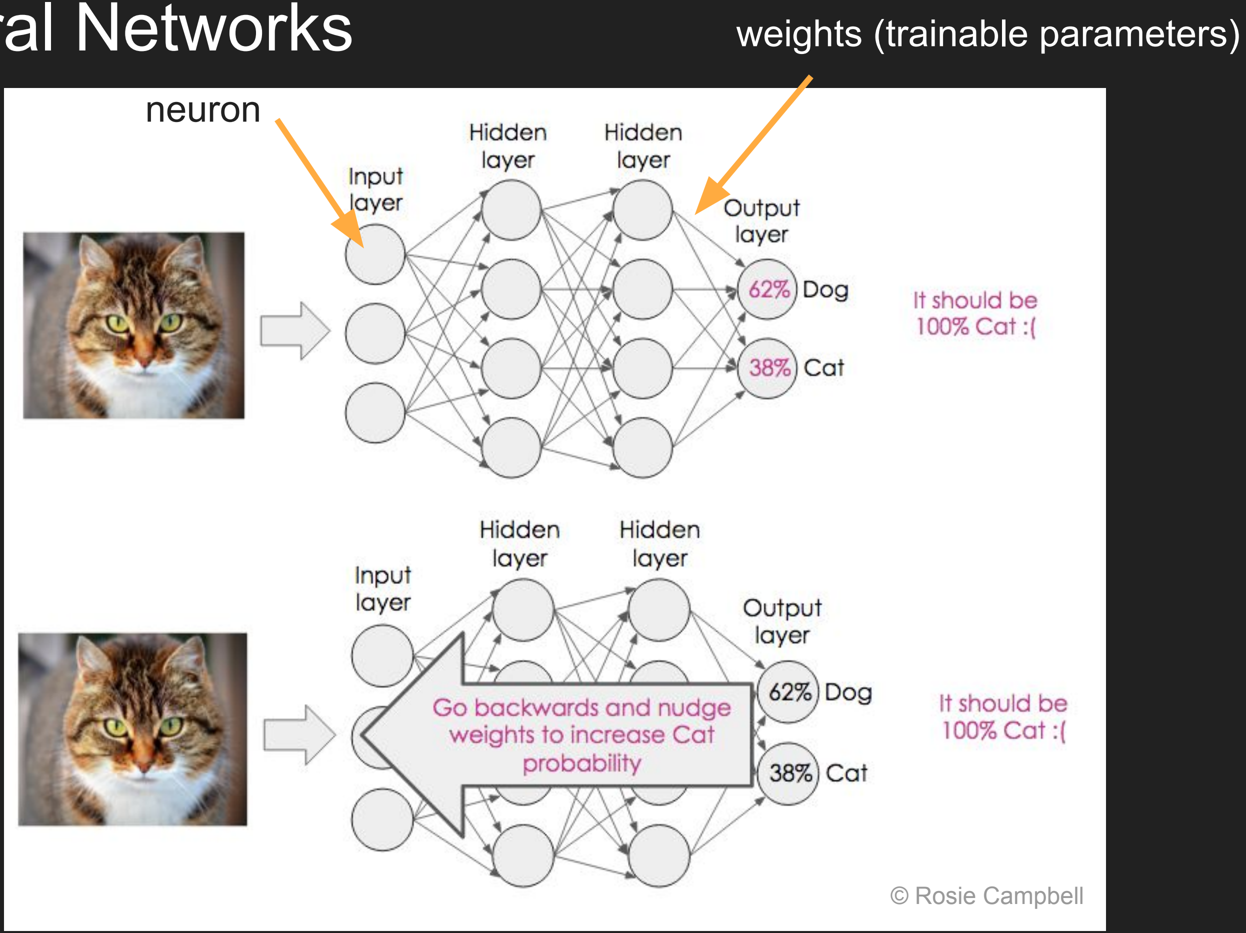
AIM

reduce to zero the numerical impact of integrating

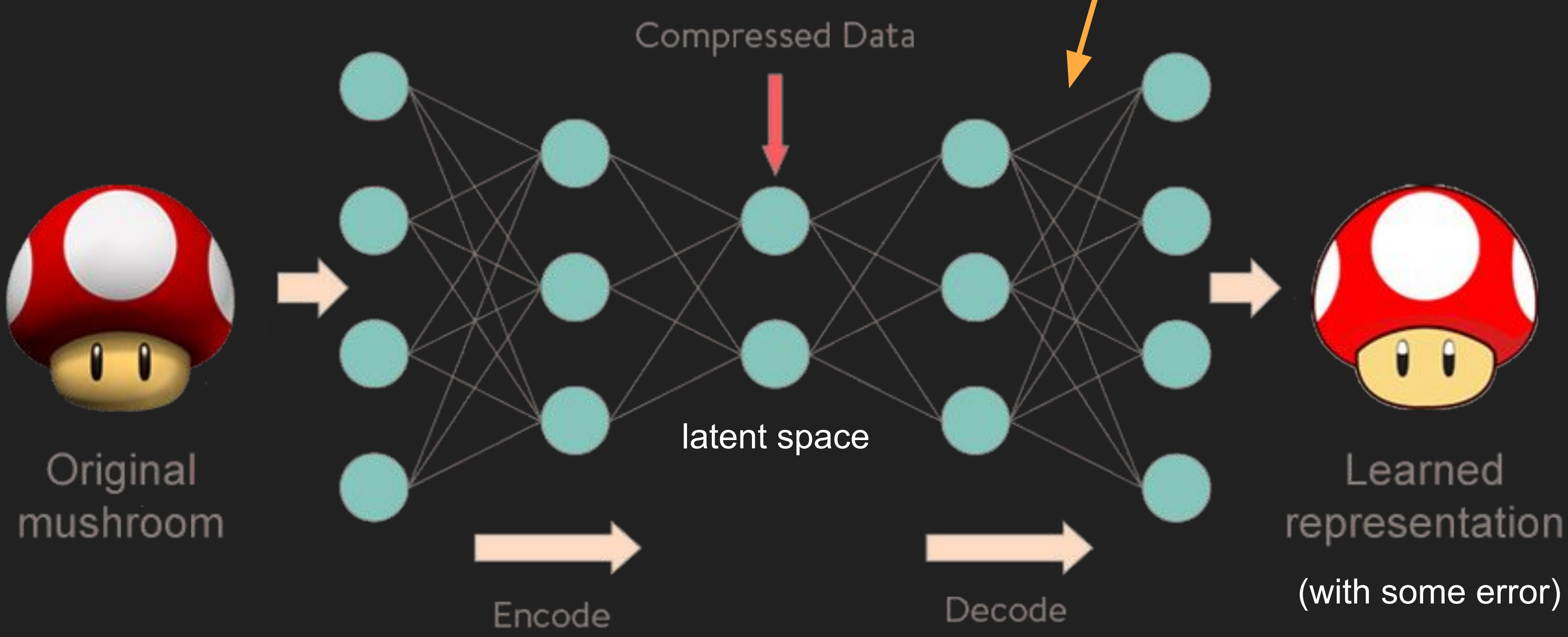
$$\dot{x} = f(\bar{x}; k)$$

with standard ODE solvers (e.g. BDF)

Deep Neural Networks



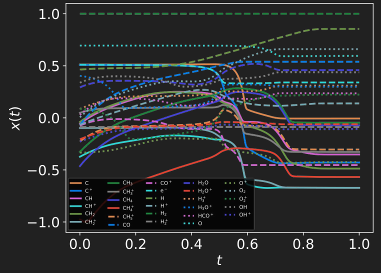
Autoencoders

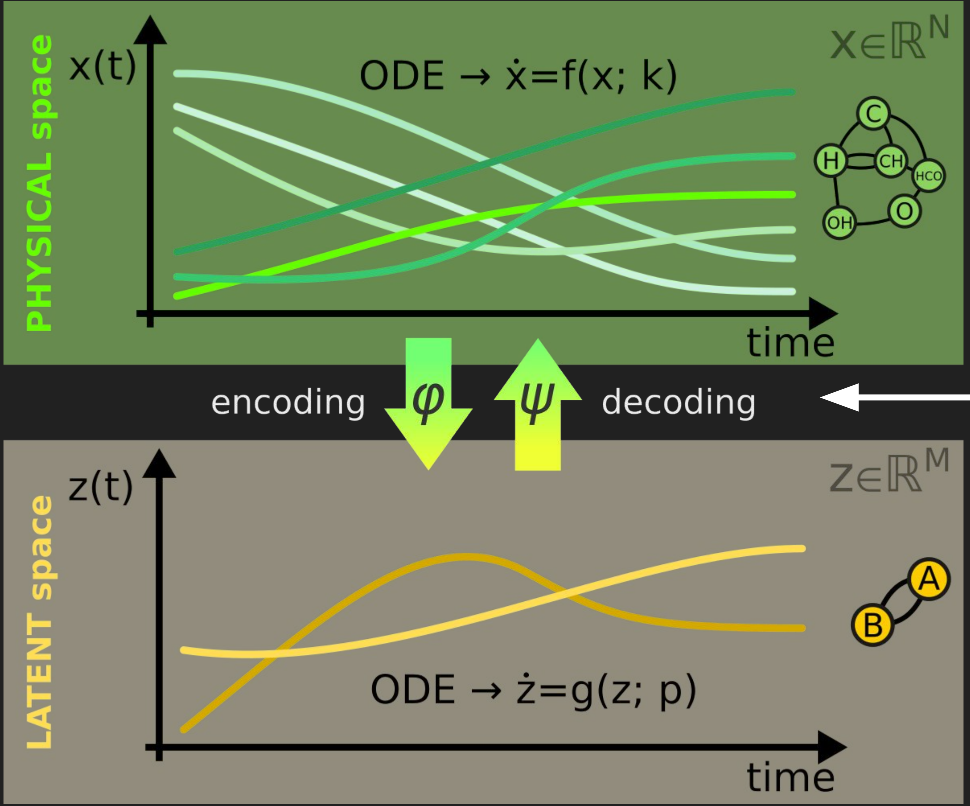


$\mathbb{R}^N$ $\mathbb{R}^{M<N}$ $\mathbb{R}^N$

AUTOENCODERS
Reduce the dimensionality of the data

Solve compressed ODE



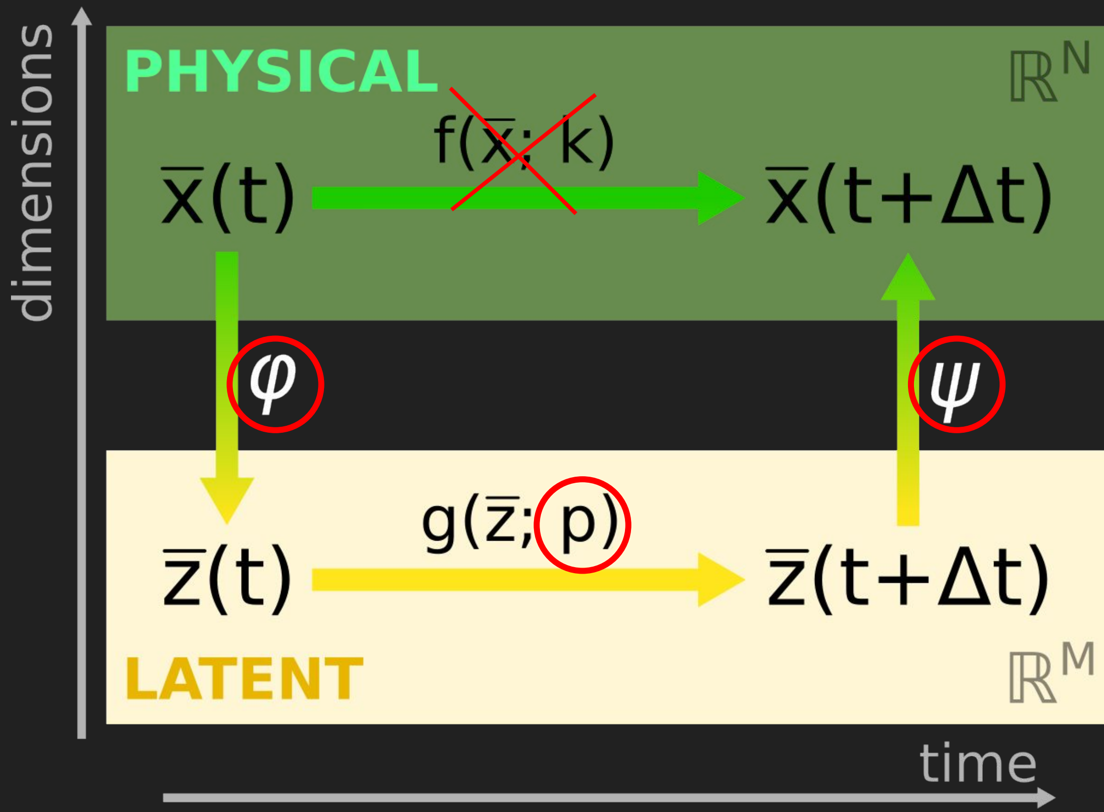


STANDARD PROBLEM

AUTOENCODER

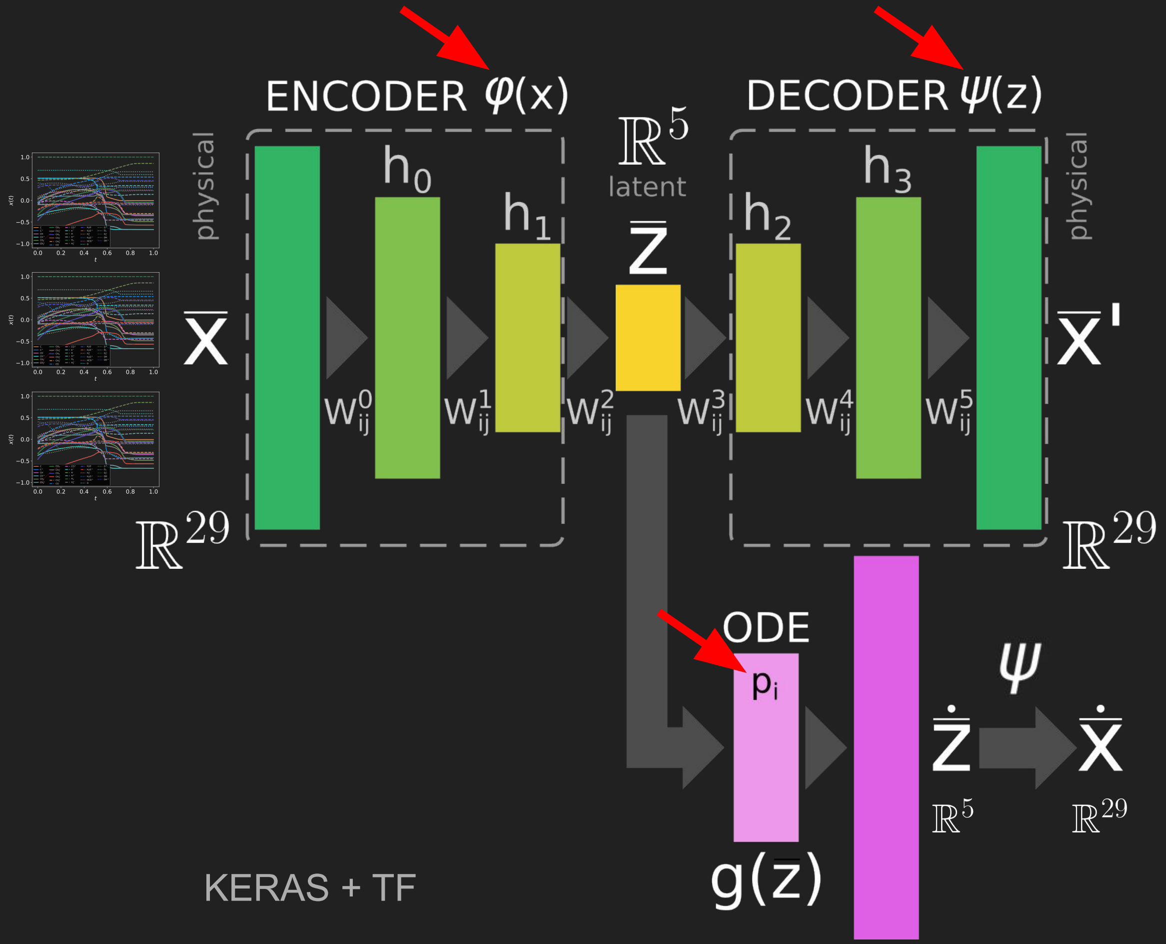
REDUCED PROBLEM

Operators



PHYSICAL
$\mathbb{R}^N$
$f(\bar{x}; k)$
$\bar{x}(t)$
$\bar{x}(t+\Delta t)$
φ
ψ
$g(\bar{z}; p)$
$\bar{z}(t)$
$\bar{z}(t+\Delta t)$
LATENT
$\mathbb{R}^M$
dimensions
time

Implementation



KERAS + TF

Latent chemical network
5 species + 12 reactions

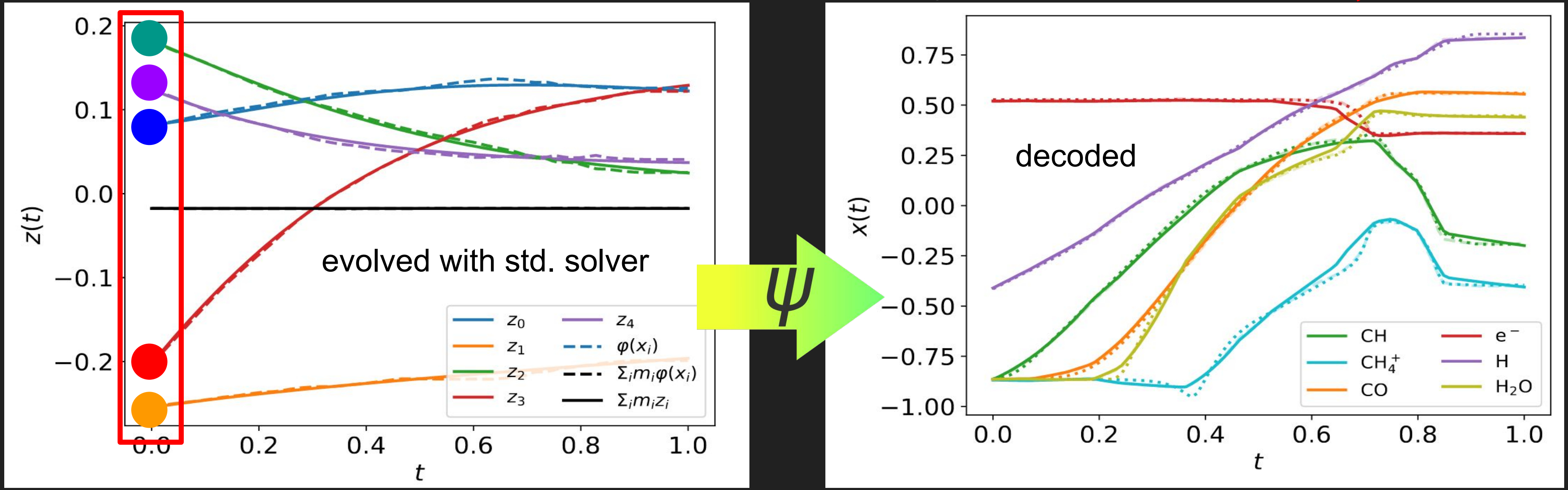
$$A + A \underset{}{\overset{p1,\, p2}{\rightleftharpoons}} AA$$
$$A + B \overset{p3,\, p4}{\rightleftharpoons} AB$$
$$B + B \overset{\dots}{\rightleftharpoons} BB$$
$$AA + BB \rightleftharpoons AB + AB$$
$$AA + B \rightleftharpoons AB + A$$
$$BB + A \rightleftharpoons AB + B$$

Original chemical network
29 species + 224 reactions

Example Results

Latent space $g(z;p)$

Physical space ~~$f(x;k)$~~



5 out of 5 “species” (A, B, AA, BB, AB)

6 out of 29 species (H, C, O, CO, CH, …)

Conclusions

Advantages:

- x65 speed-up (but in practice: integration time $\longrightarrow 0$)
- Interpretability of the latent space (it's a chemical network!)
- New perspective on the problem
- Promising (we also might learn something from latent space)

Limitations:

- $g(z; p)$ needs to be designed beforehand (but…)
- It needs training data
- This case-study uses constant temperature, CRs, radiation, ...
- Training needs some fine-tuning
- Is the compression always guaranteed? We don't know