Lessons from Physics-Informed Neural Networks:

Inverse Problems Across Phase Transitions

3rd International Workshop on AI + Astronomy: Models, Data, Discovery
Zhejiang Lab, Hangzhou · October 2026

Based on 2403.14763, 2606.30117
and work in progress

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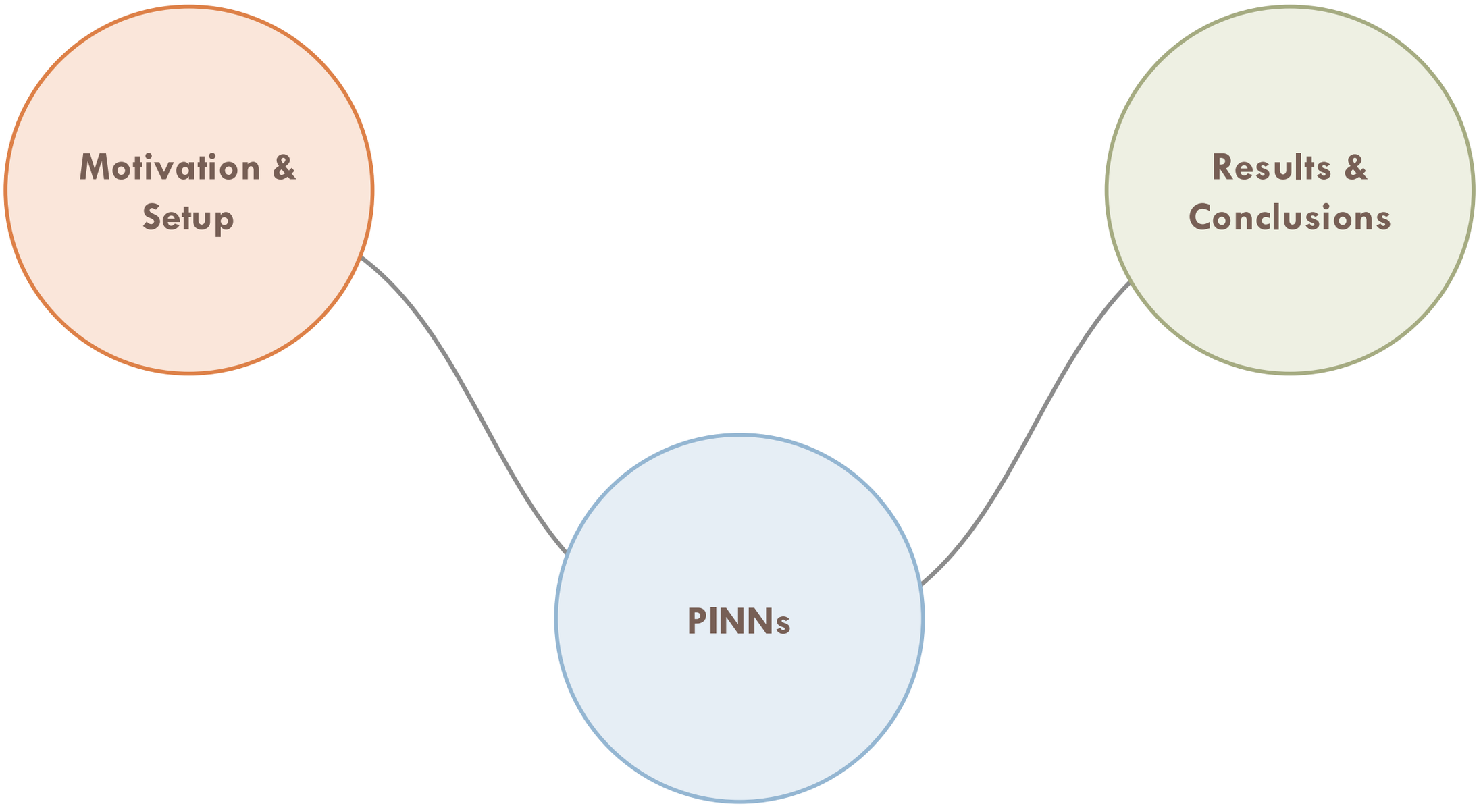
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EXCELENCIA MARÍA DE MAEZTU 2020–2024

Roadmap



Roadmap

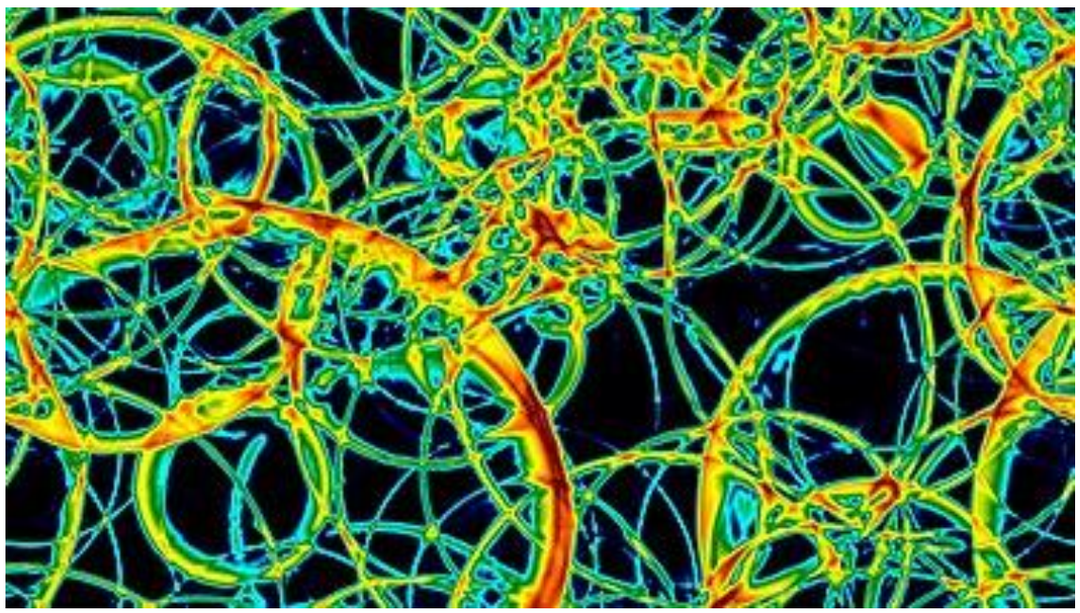
Motivation & Setup

- Early-Universe phase transitions
- Holography: real-time, strongly-coupled dynamics
- The inverse problem

PINNs

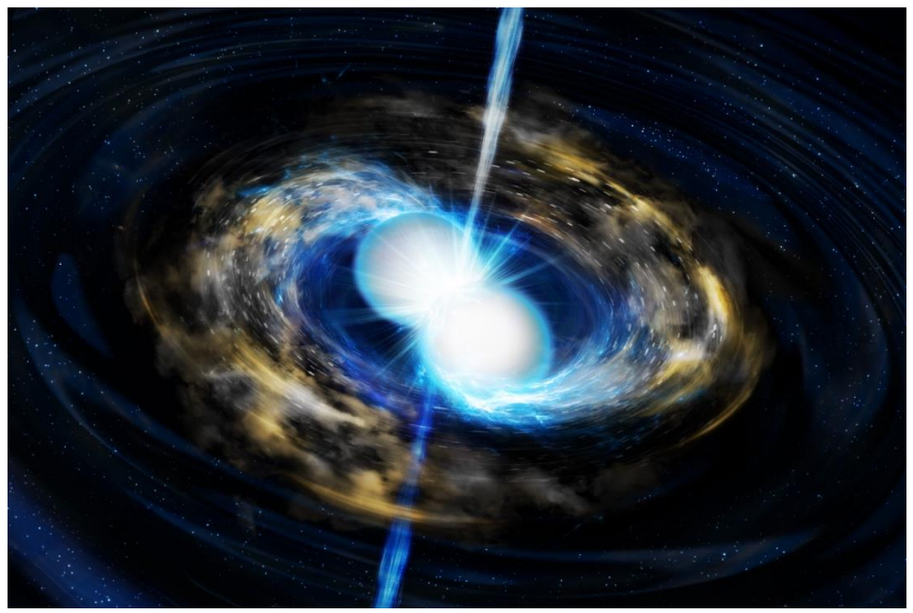
Results & Conclusions

Phase transitions in the Universe



Early Universe

- Standard-Model transitions are crossovers, but many extensions predict **first-order** ones
- Evidence of **BSM**



Neutron-star mergers

- A first-order QCD transition at high density nucleates bubbles in the remnant
- **SM** in unexplored regime

Cosmological/astrophysical data to fundamental physics

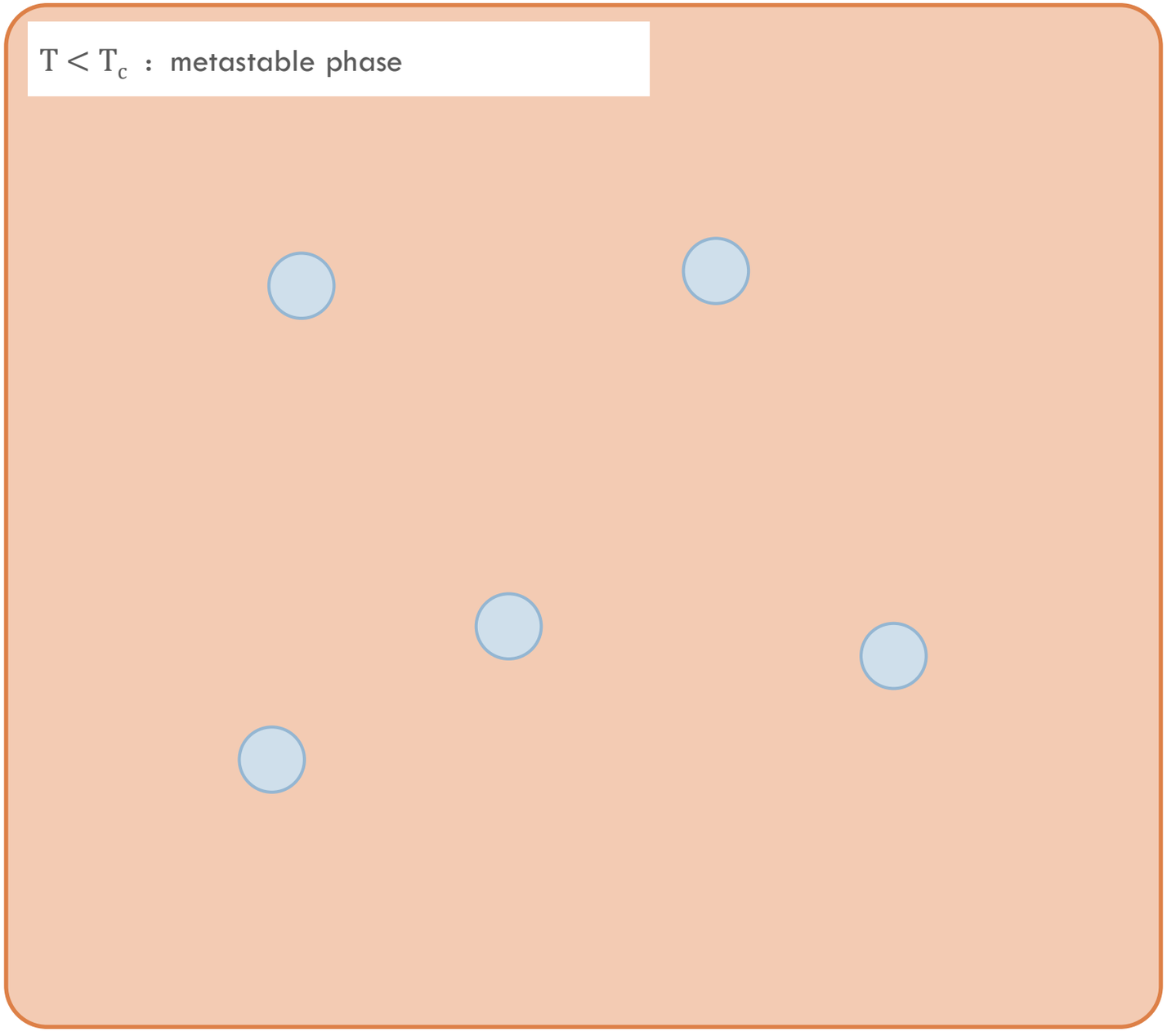
Bubbles ⟶ gravitational waves

$T < T_c$: metastable phase

Supercooling

- Below T_c the plasma can stay in the **metastable** phase

Bubbles ⟶ gravitational waves

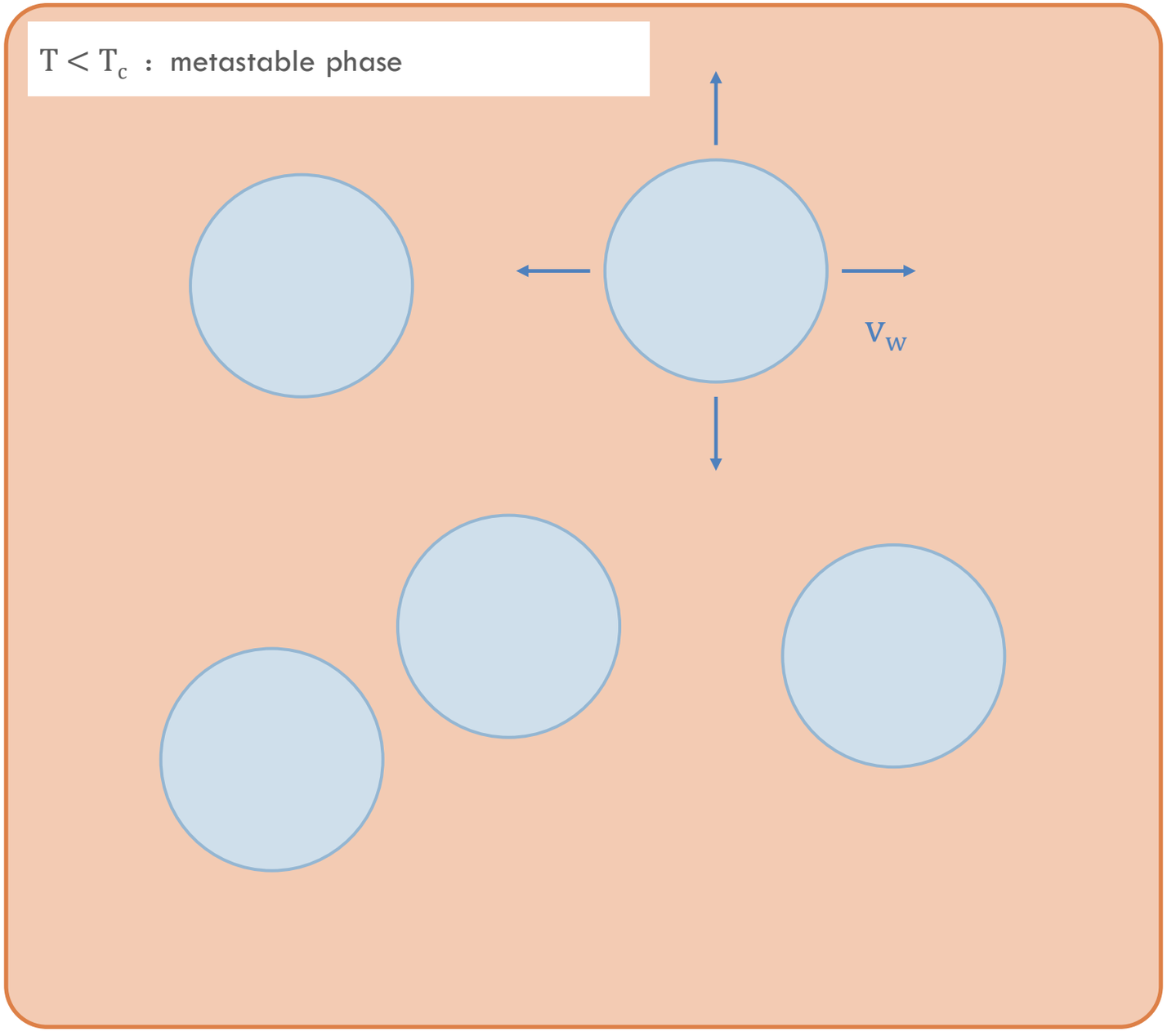


Nucleation

- The transition proceeds via **bubble nucleation**
- Bubbles of the new stable phase appear from random thermal fluctuations

  Bea et al. '22 (2202.10503)

Bubbles ⟶ gravitational waves

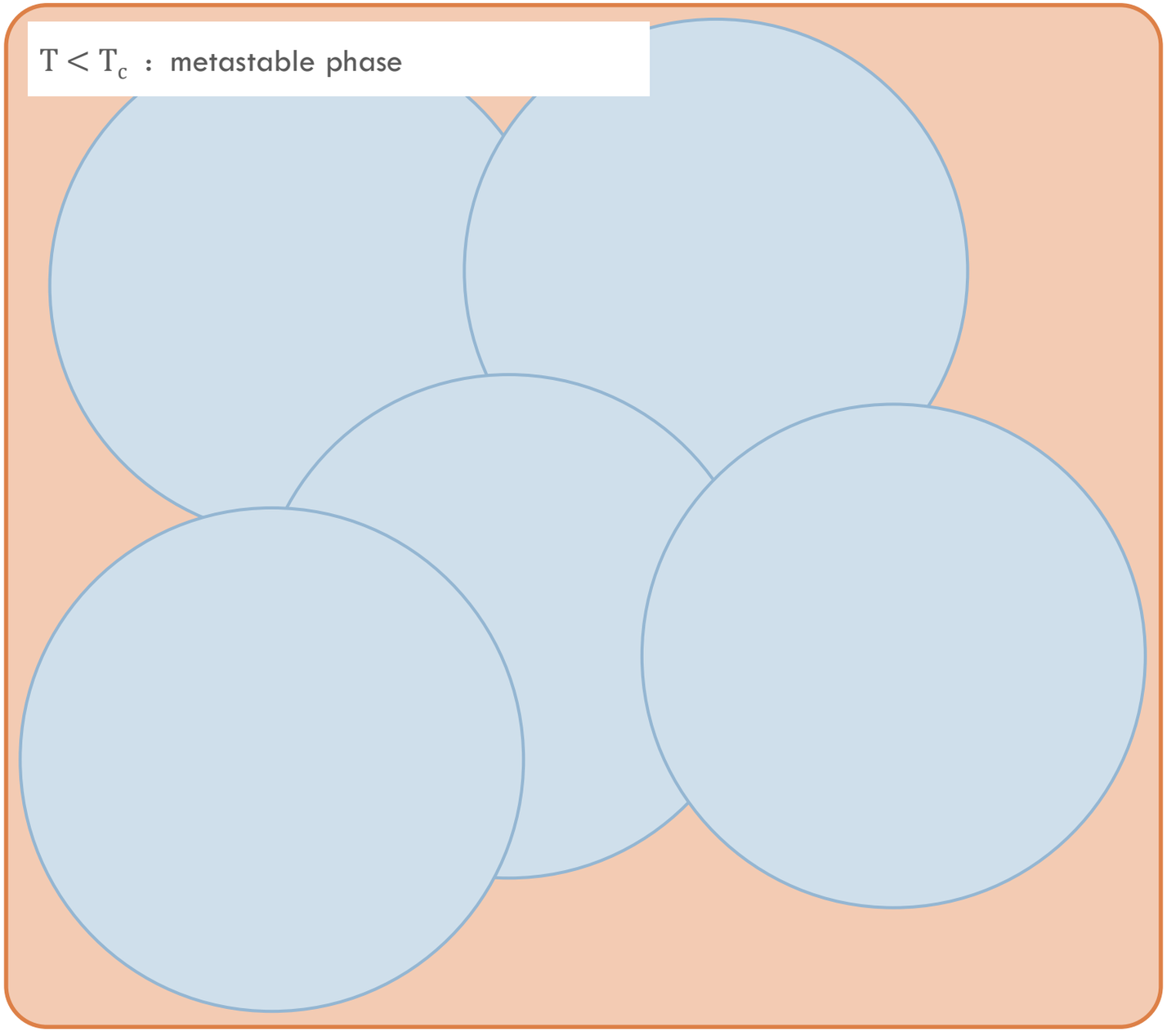


Expansion

- Walls accelerate to a **terminal velocity**
- The plasma is pushed around, hydrodynamics works away from the wall

  Bea et al. '21 (2104.05708)

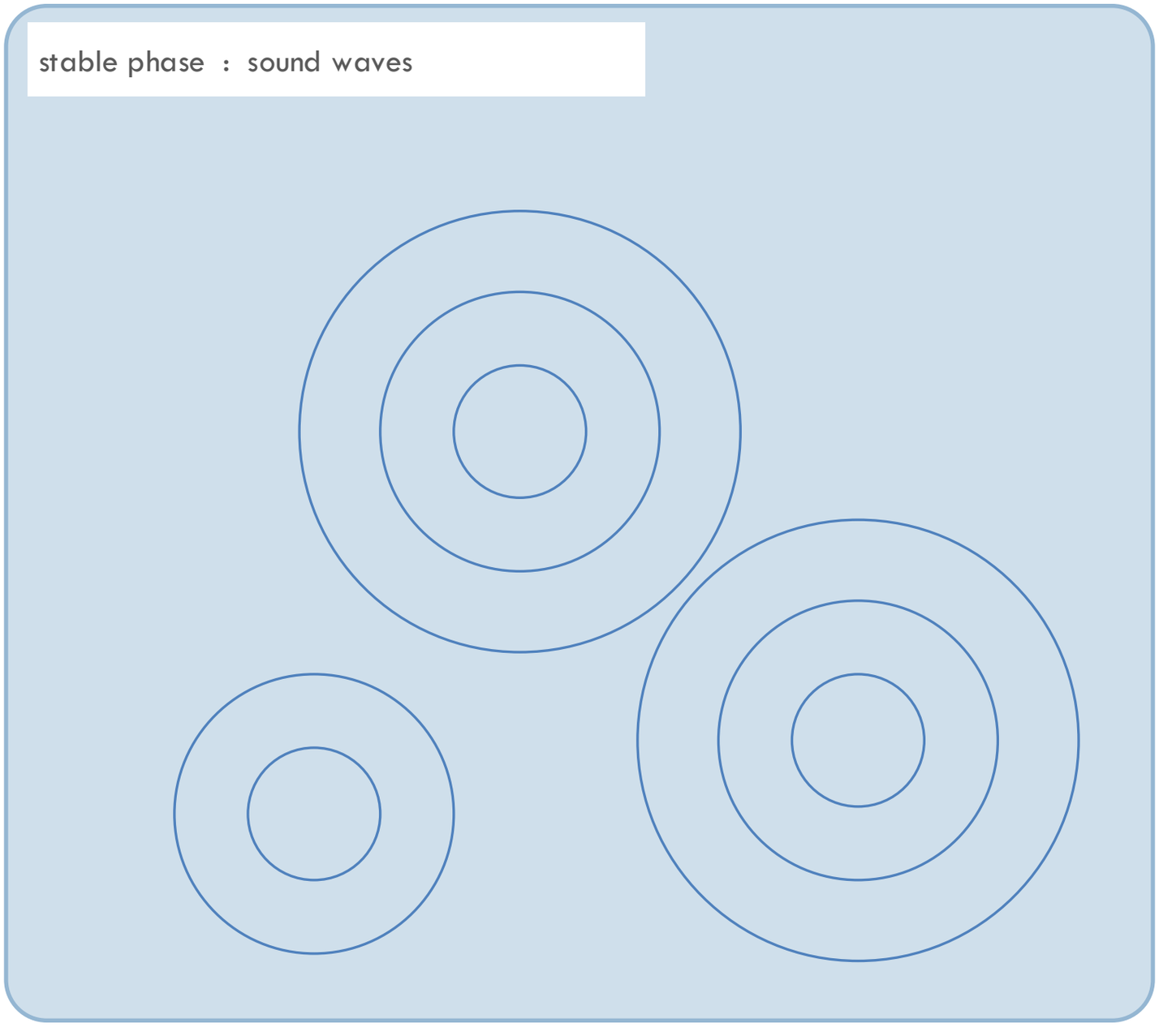
Bubbles ⟶ gravitational waves



Collisions

- Bubbles merge, the energy of the walls goes into **sound waves** in the plasma

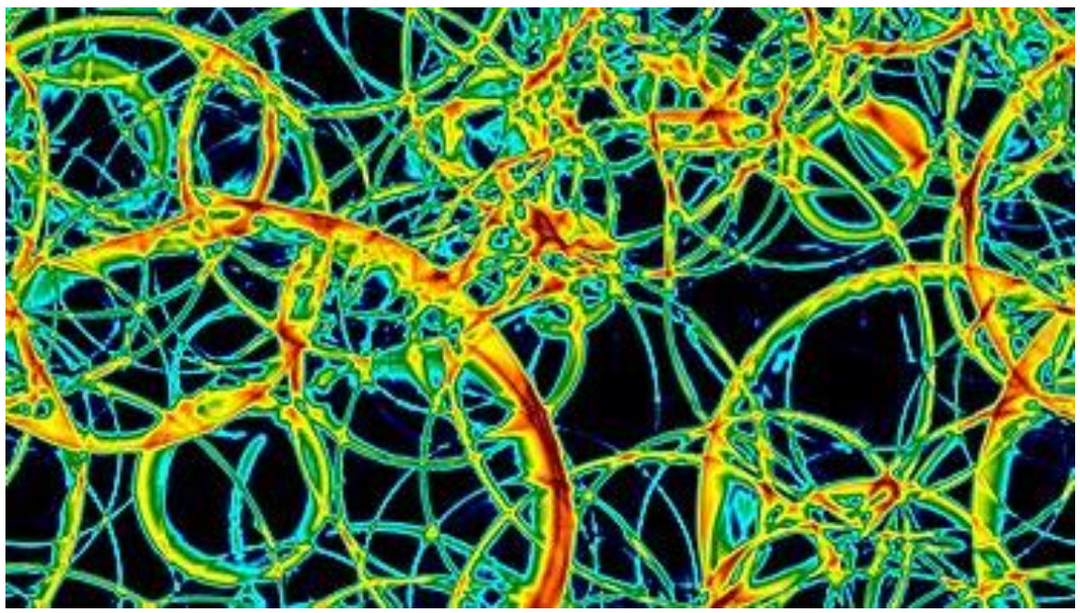
Bubbles → gravitational waves



Gravitational waves

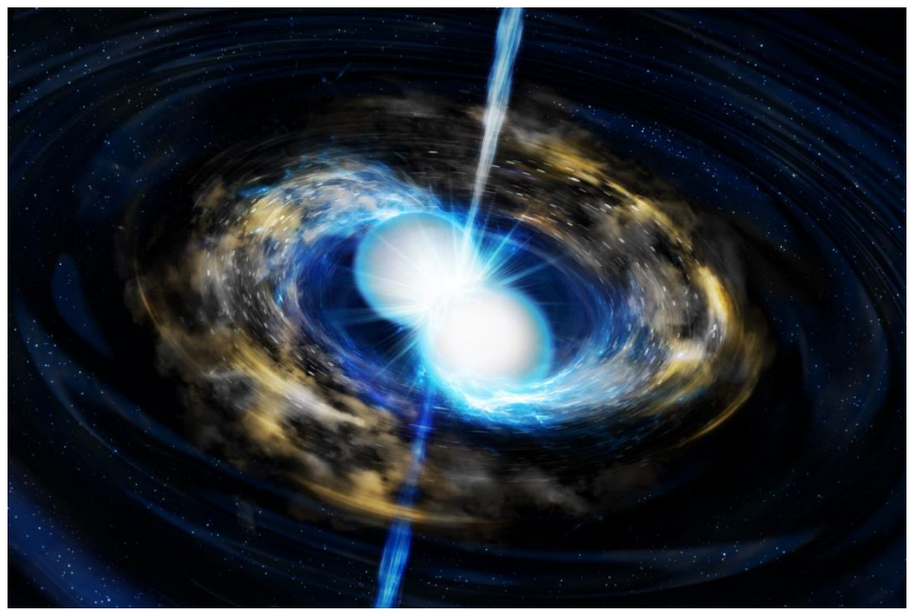
- Sound waves source a stochastic **GW background**
- Peak frequency & amplitude set by various **model parameters** (ex: nucleation temperature, bubble wall velocity…)

Phase transitions in the Universe



Early Universe

- Stochastic GW background in the **mHz** band: **LISA, Taiji, TianQin**



Neutron-star mergers

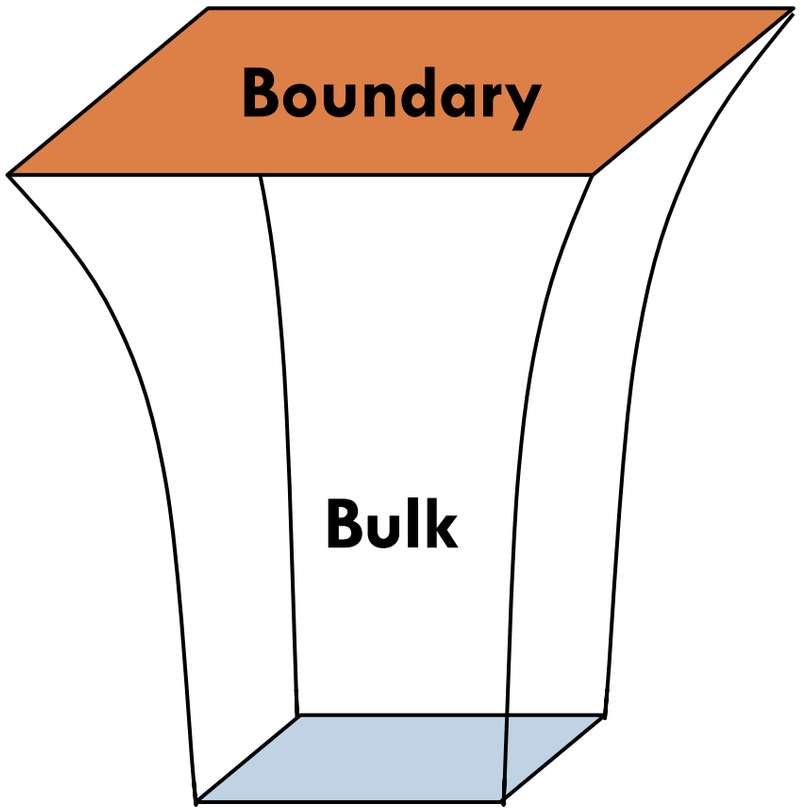
- Gravitational waves in the **MHz** band (only known astrophysical source within SM) Blas, Casalderrey-Solana, Mateos, Sanchez-Garitaonandia '22

- To predict the spectrum we need model parameters

In both cases the matter is **strongly coupled** and **far from equilibrium**

→ Holography

Holography in a nutshell

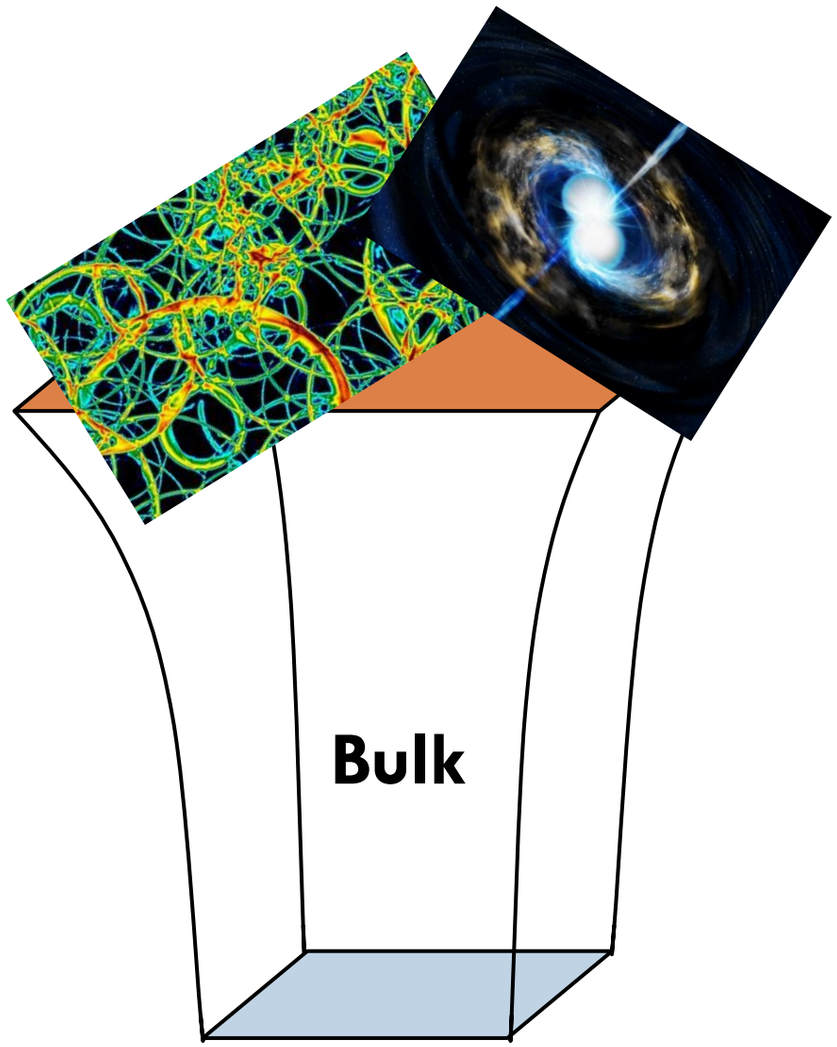


Quantum field theory in **4D**

Classical gravity in **5D** anti-de Sitter spacetime

Holography in a nutshell

Strongly coupled
(“**difficult**”)

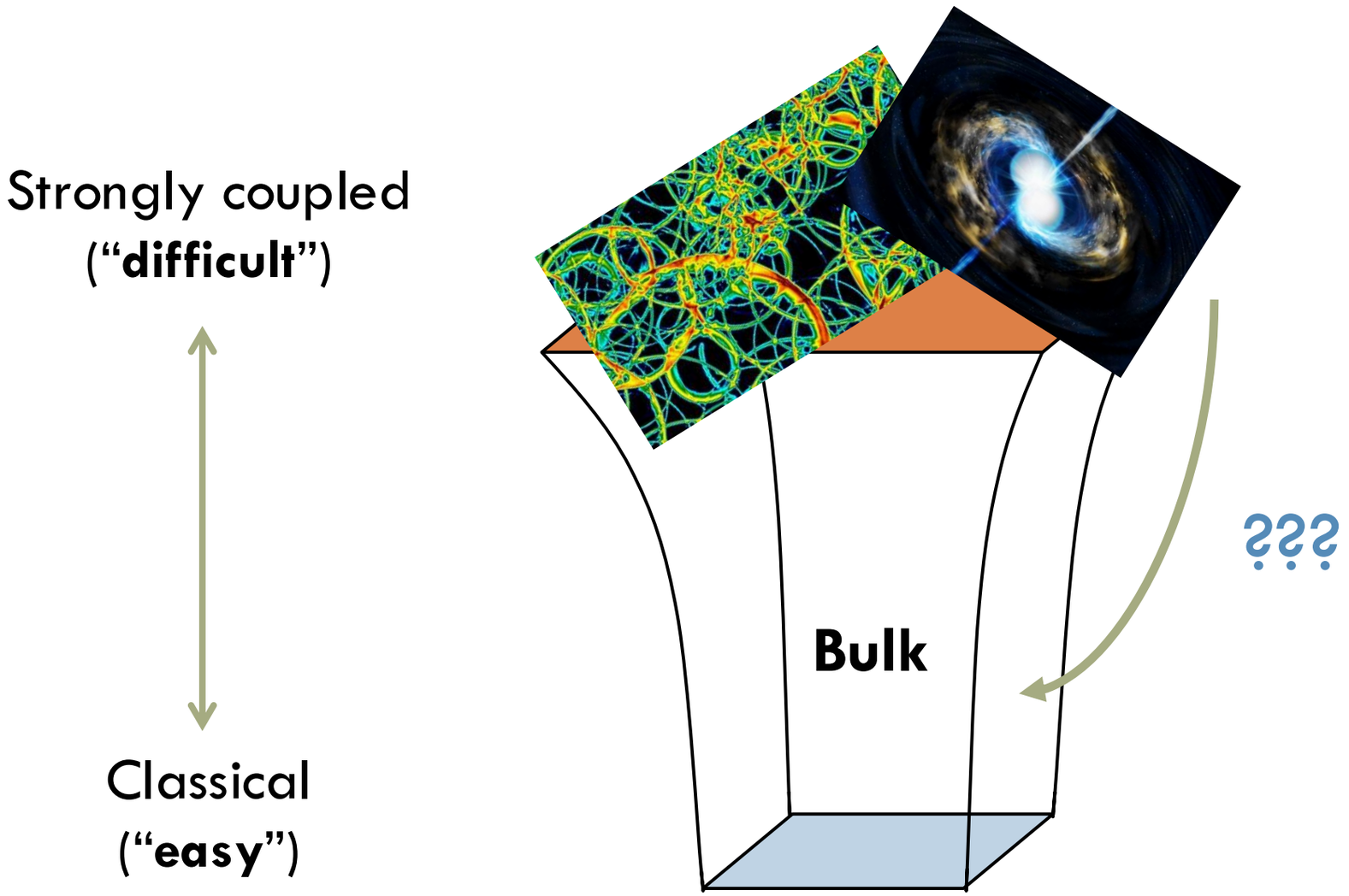


Numerical simulation tool

Classical
(“**easy**”)

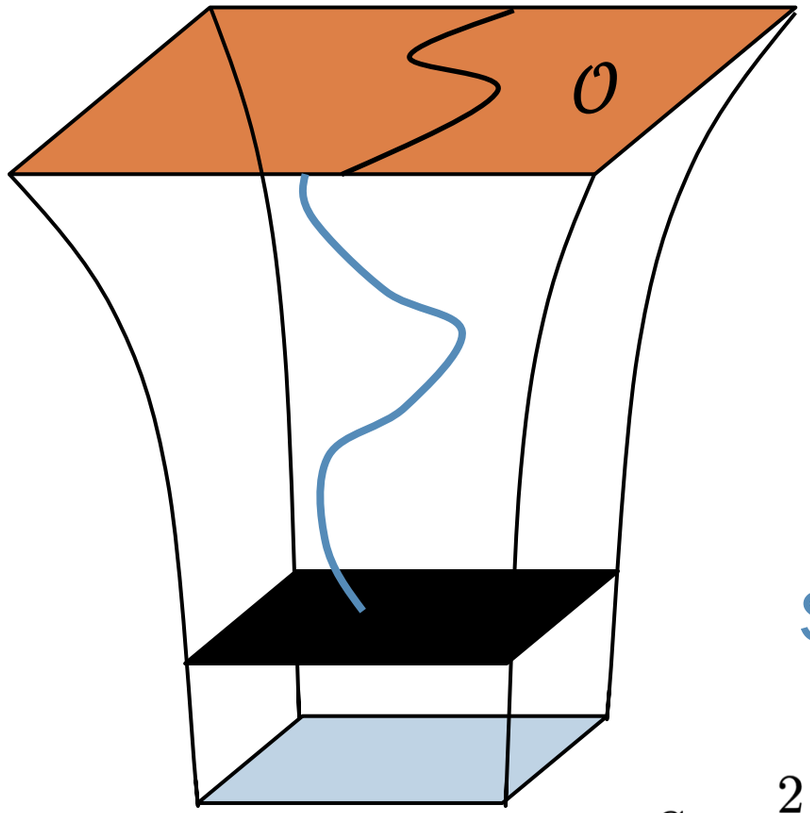
- Far-from-equilibrium dynamics by **evolving the gravity side** (can be used to simulate bubble nucleation), not possible using lattice formulation

Holography in a nutshell



- Far-from-equilibrium dynamics by **evolving the gravity side** (can be used to simulate bubble nucleation), not possible using lattice formulation

Holography in a nutshell



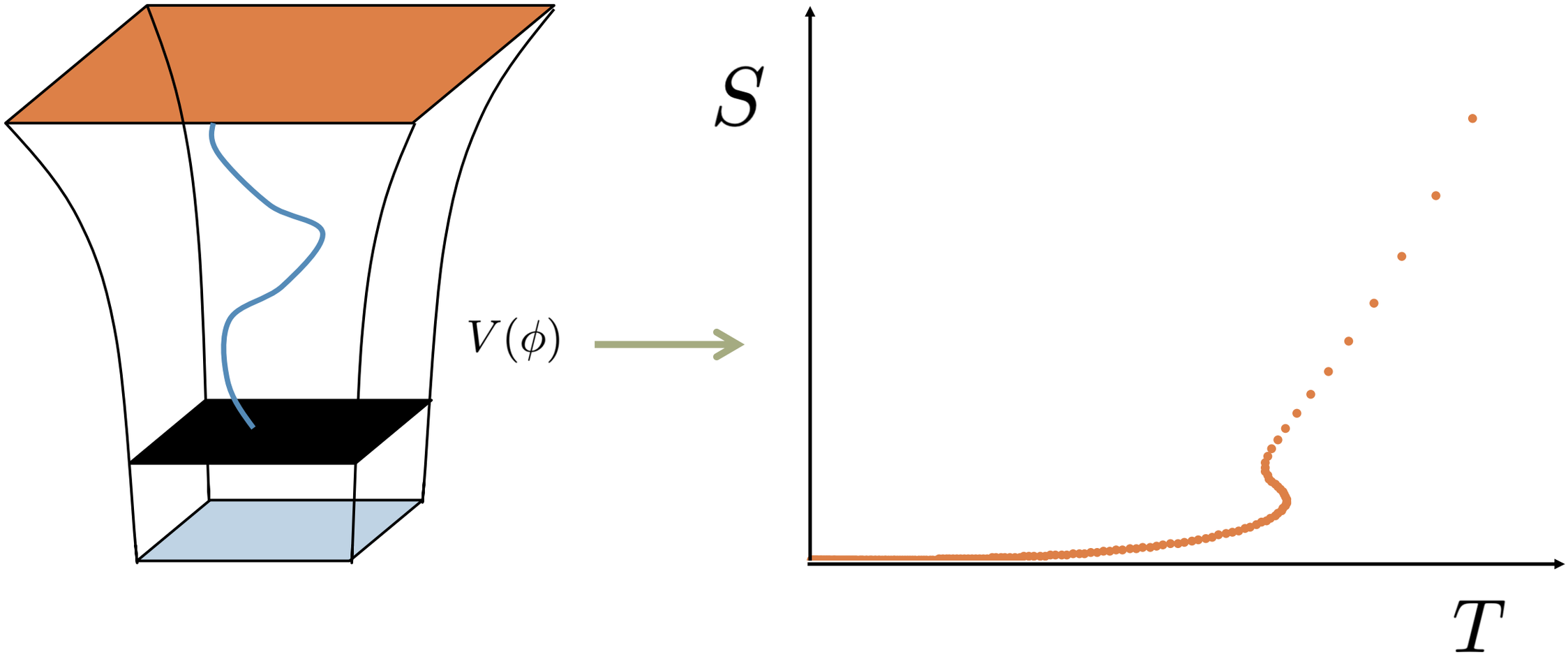
Phase transition

Scalar field potential $V(\phi)$

$$S = \frac{2}{\kappa_5^2}\int dx^5\sqrt{-g}\left[\frac{1}{4}R - \frac{1}{2}(\nabla\phi)^2 - V(\phi)\right]$$

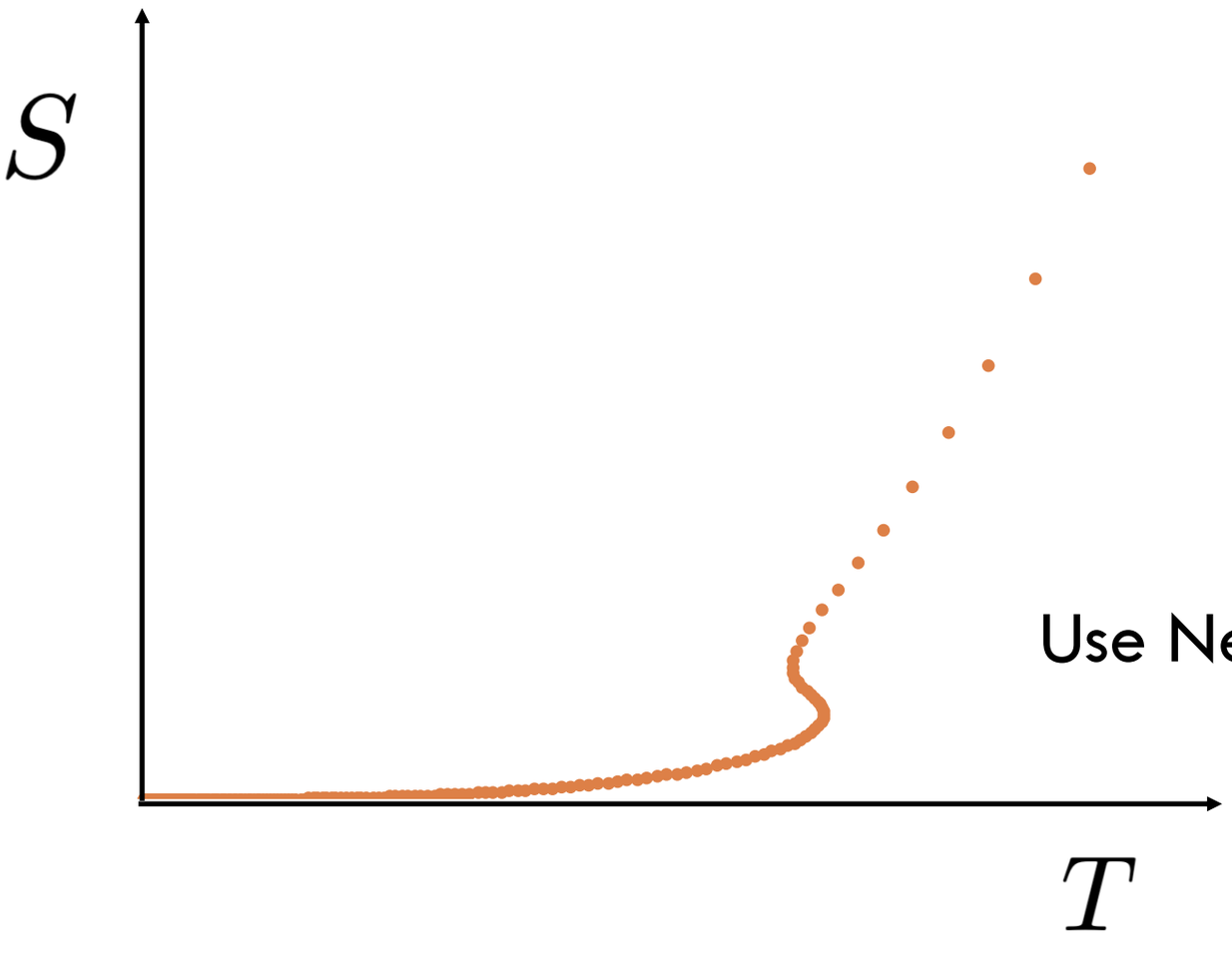
- Gravity theory is **entirely characterized** by $V(\phi)$

Direct vs inverse problem

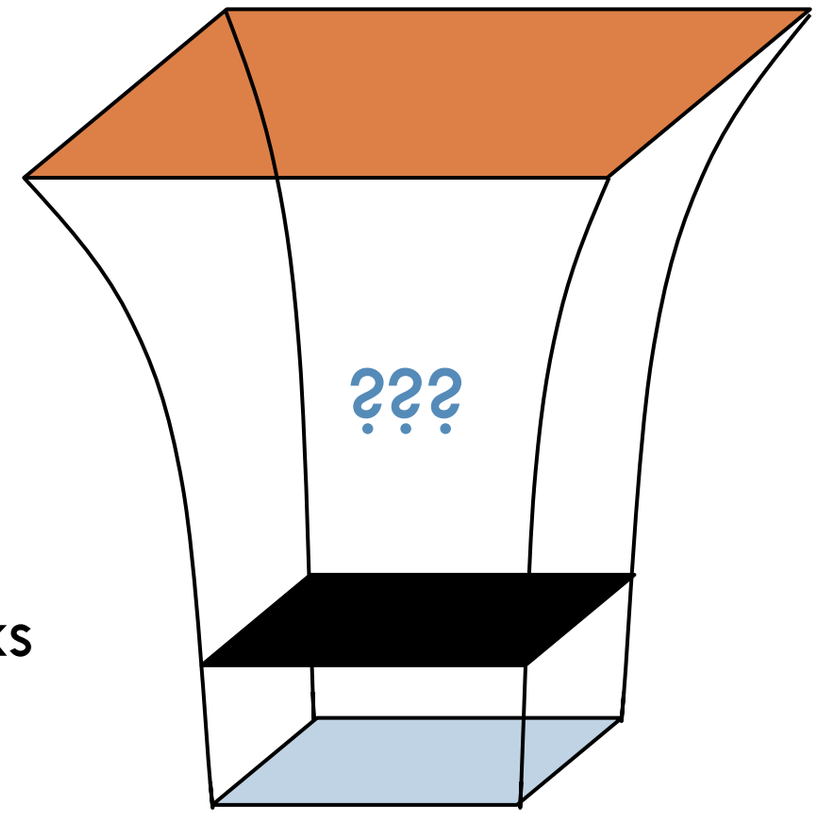


Direct problem

Direct vs inverse problem

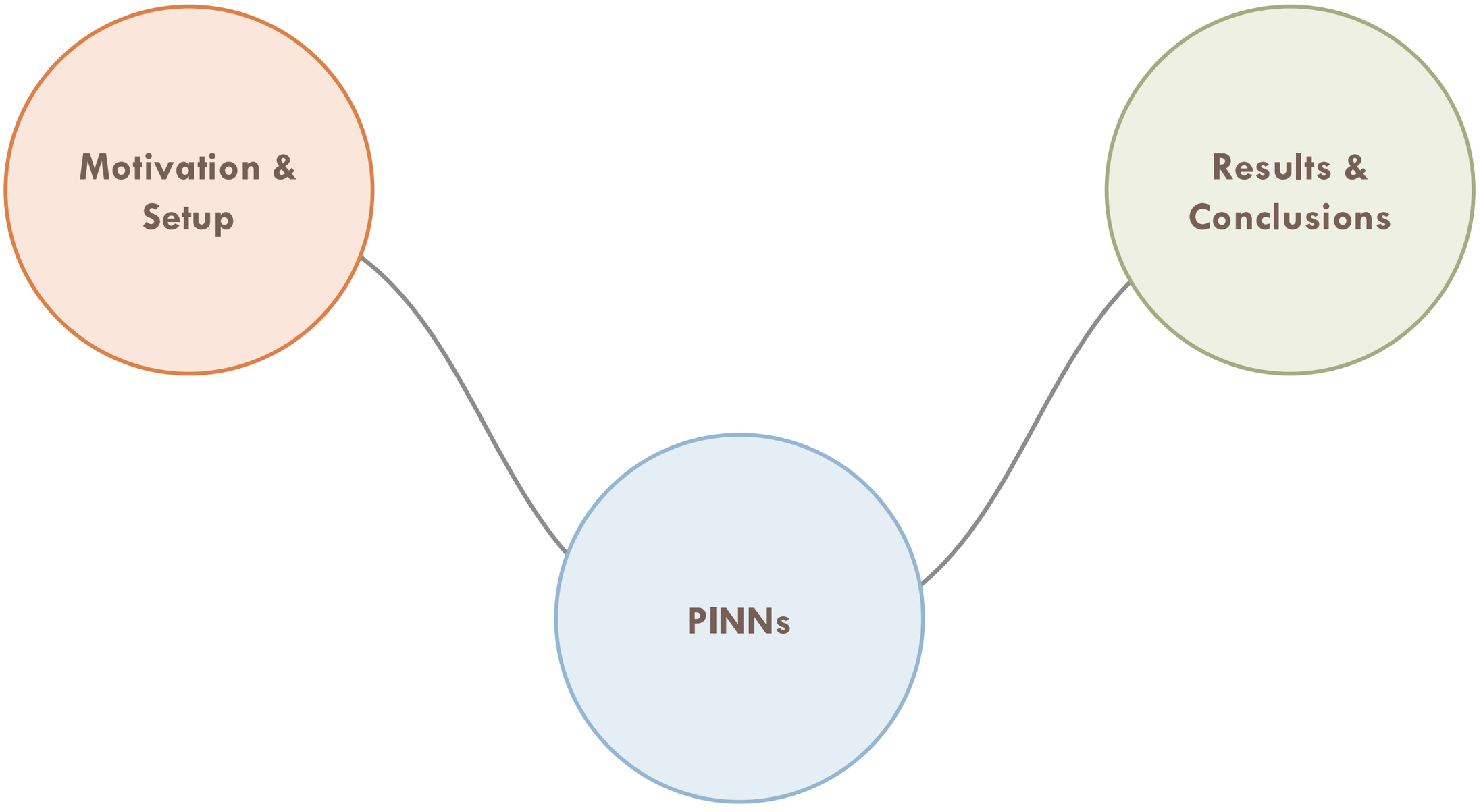


Use Neural Networks

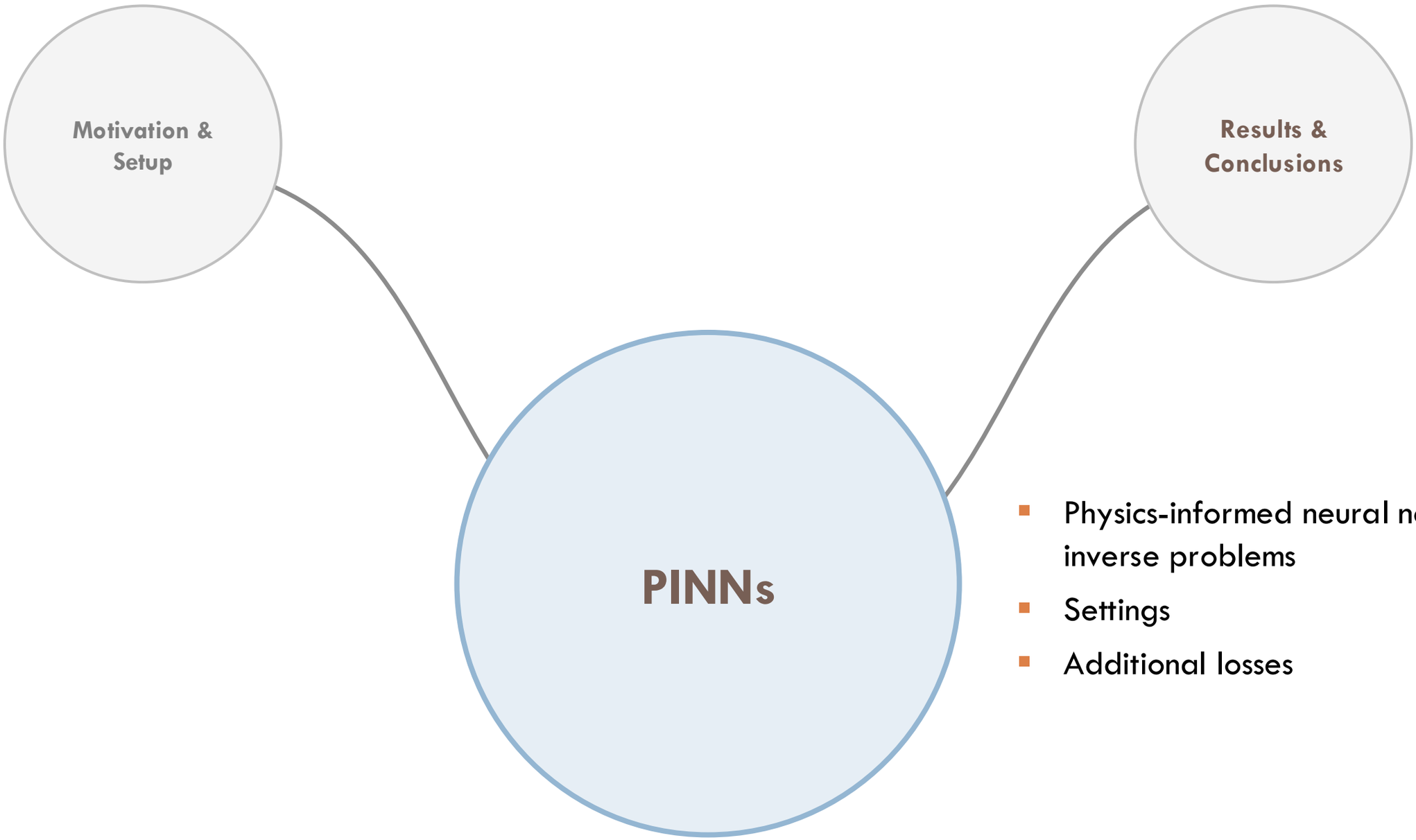


Inverse problem

Roadmap



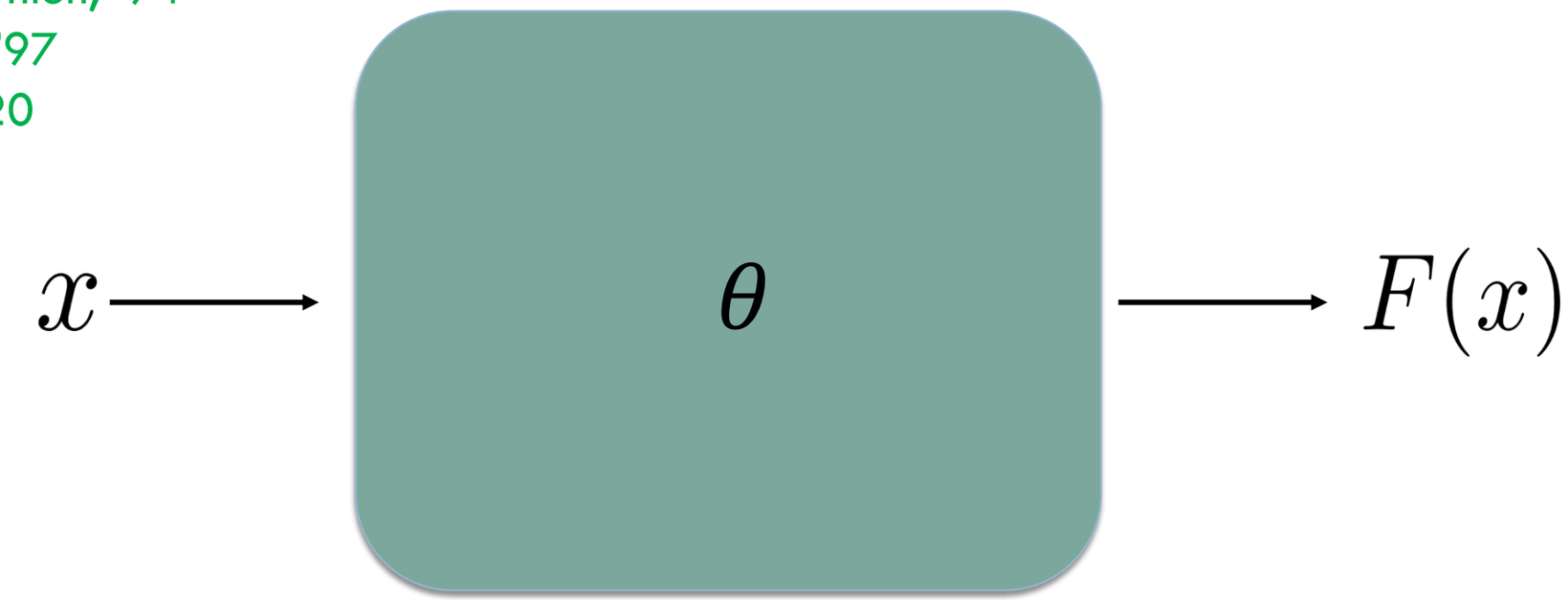
Roadmap



- Physics-informed neural networks for inverse problems
- Settings
- Additional losses

Physics-Informed Neural Networks

Dissanayake, Phan-Thien, '94
Lagaris et al, '97
Chen et al, '20

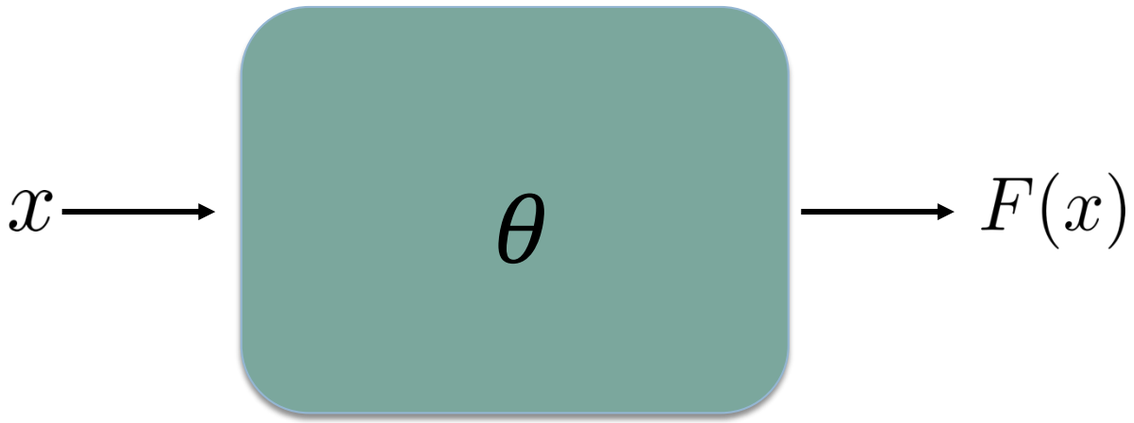


$$\mathcal{L}(\theta) = \frac{1}{N}\sum_{\mu}\sum_{i=1}^{N}\left|\mathcal{D}\,\psi_\theta(x_i^\mu) - f(x_i^\mu)\right|^2$$

- PINNs **loss function** is defined as the **residuals of the differential equations**

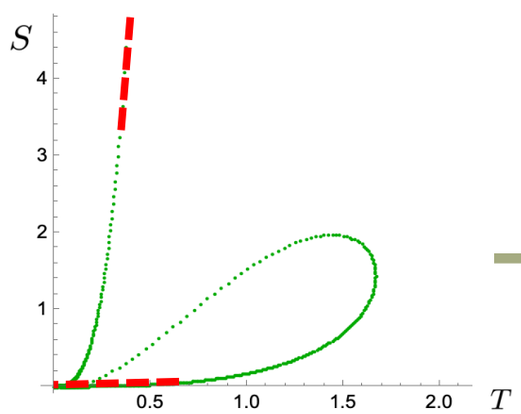
Physics-Informed Neural Networks

- Train for **many BCs at once,** satisfied by construction (the S(T) curve itself)



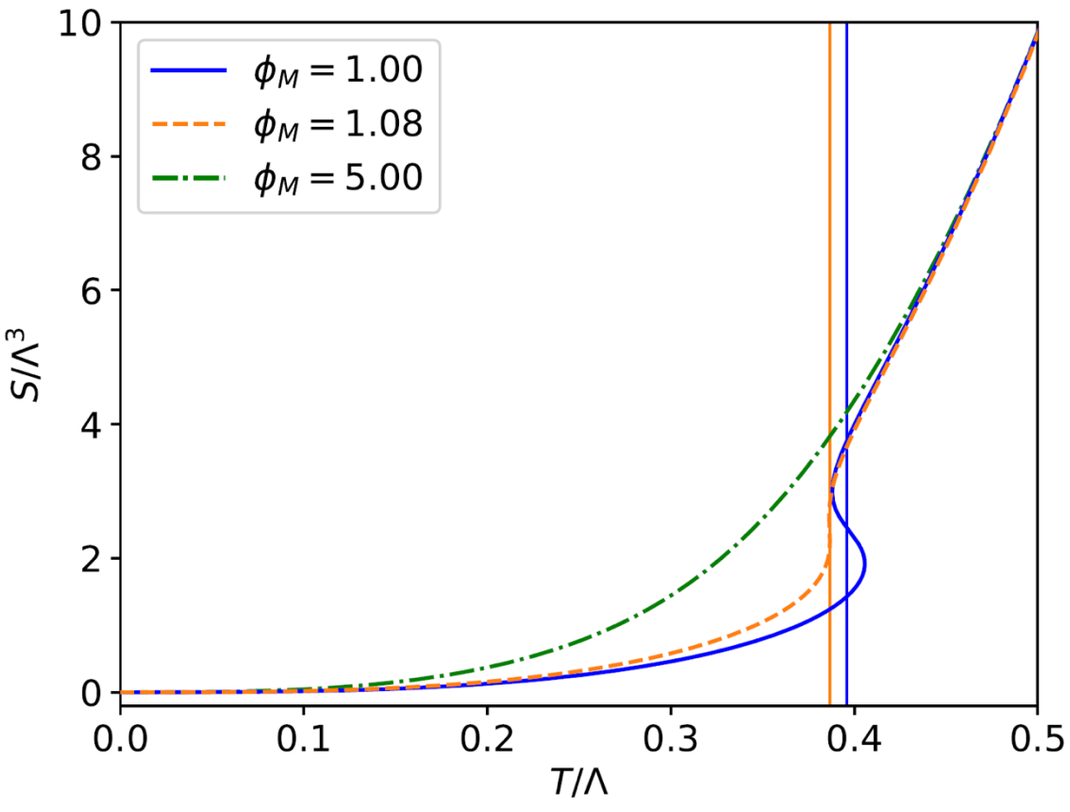
- **One network per unknown function,** no training data (evaluate on sampled points)

- Can also put **additional losses** from our Physics knowledge:



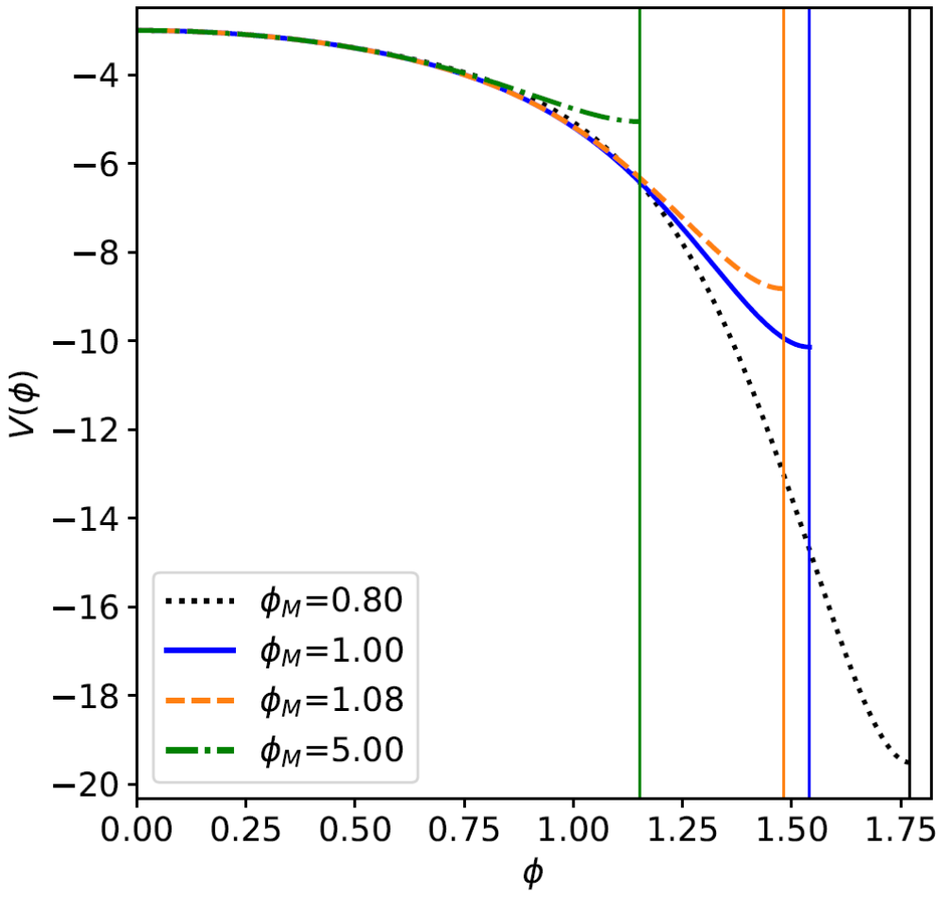
$$S \propto T^3$$

The task at hand

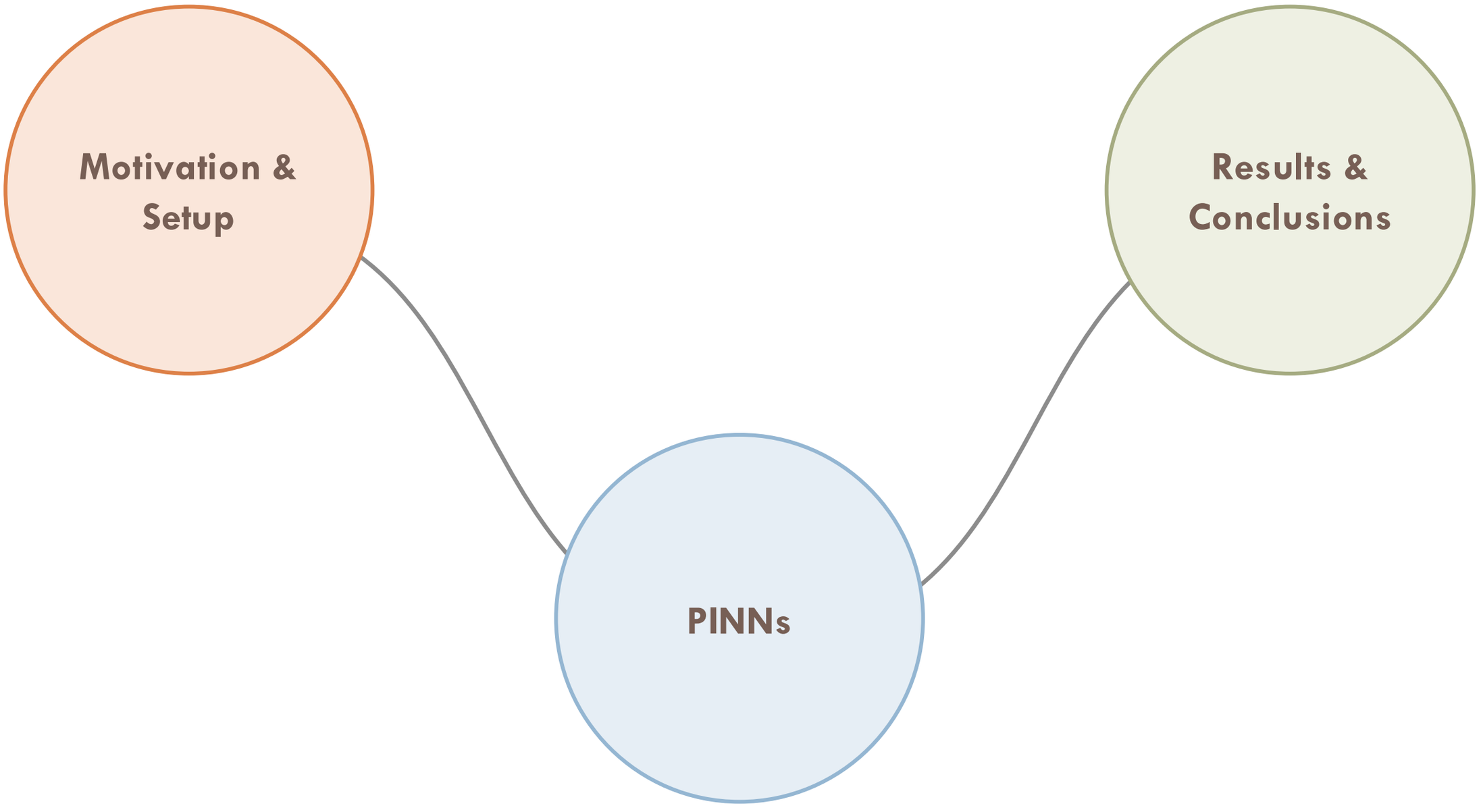


Inverse problem:
PINNs

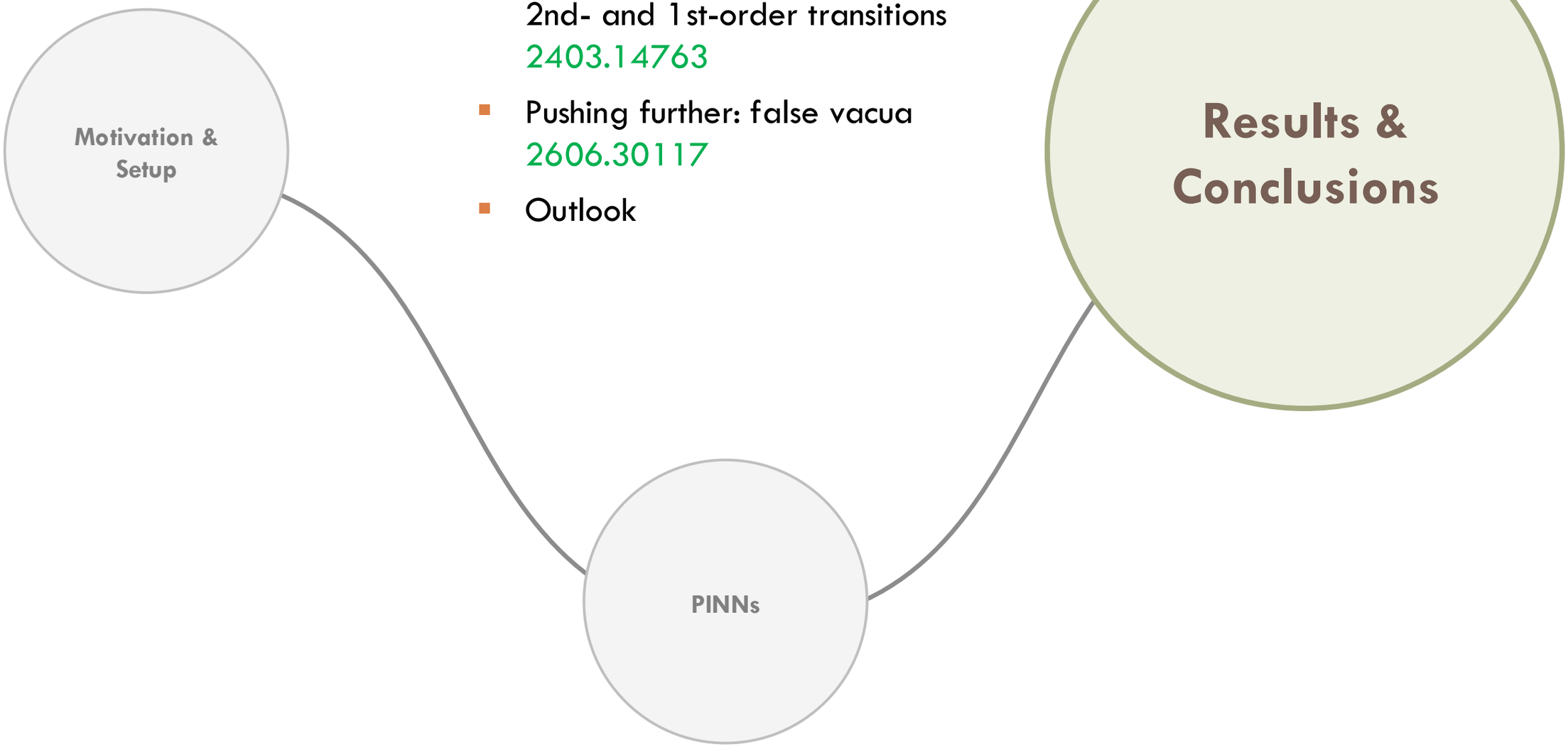
Direct problem:
Compare S(T)



Roadmap



Roadmap

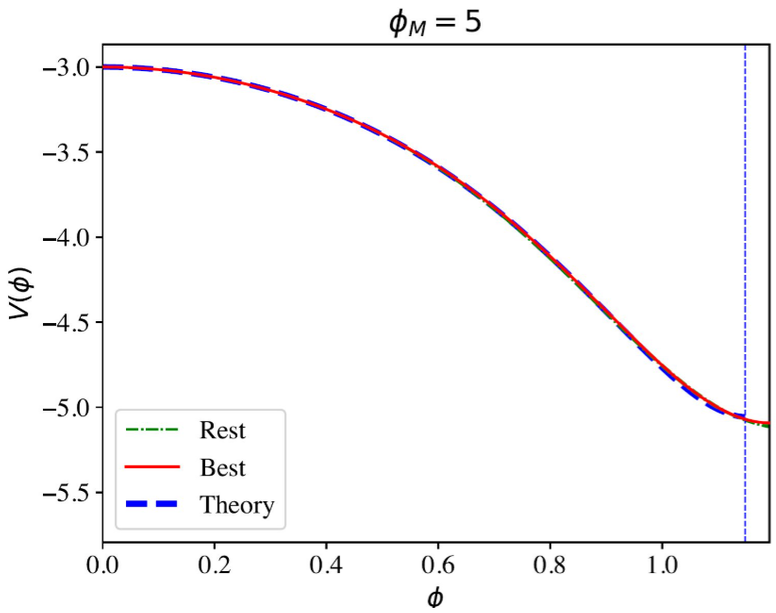


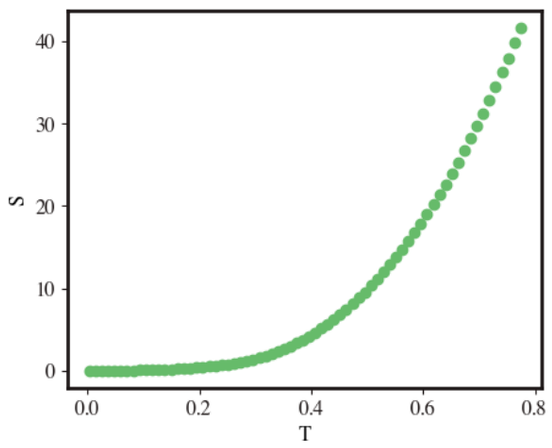
- Reconstructed potentials: crossover, 2nd- and 1st-order transitions 2403.14763
- Pushing further: false vacua 2606.30117
- Outlook

Results

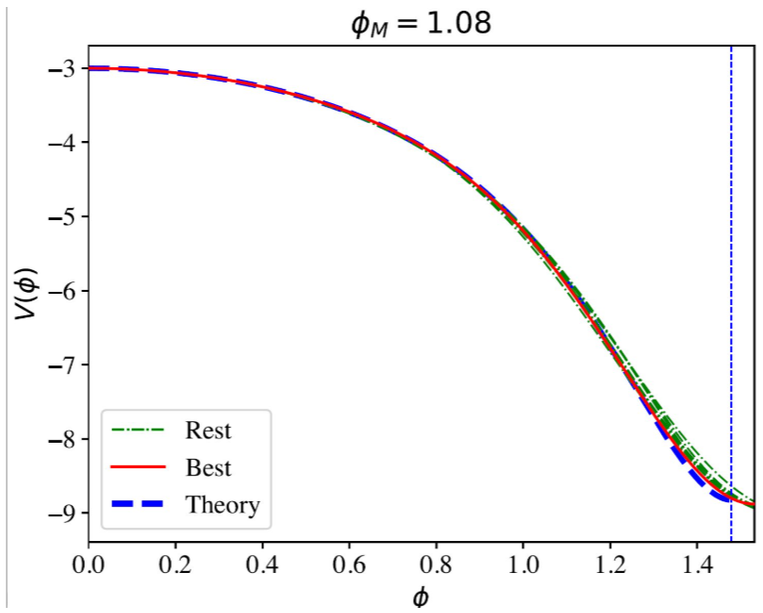
Bea, Jiménez, Mateos, Liu, Protopapas, Tarancón-Álvarez, Tejerina-Pérez ‘24

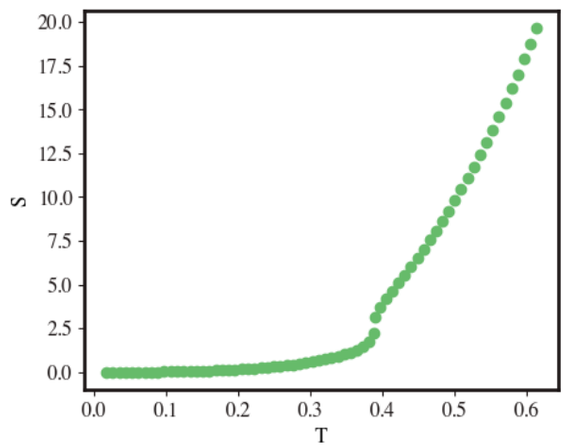
Crossover



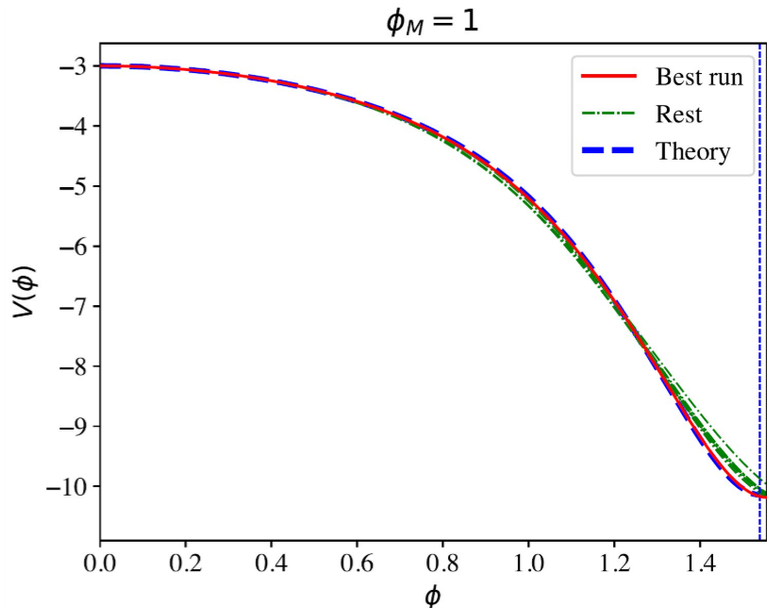


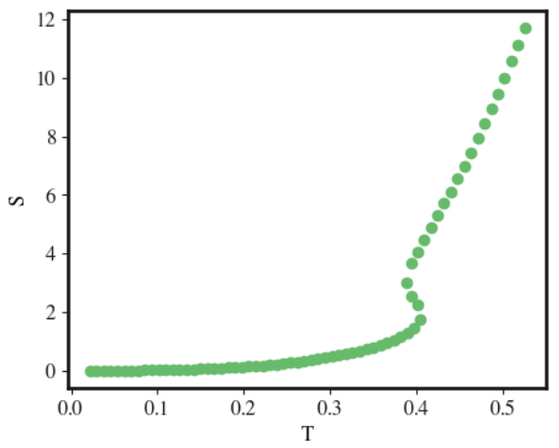
2nd order





1st order

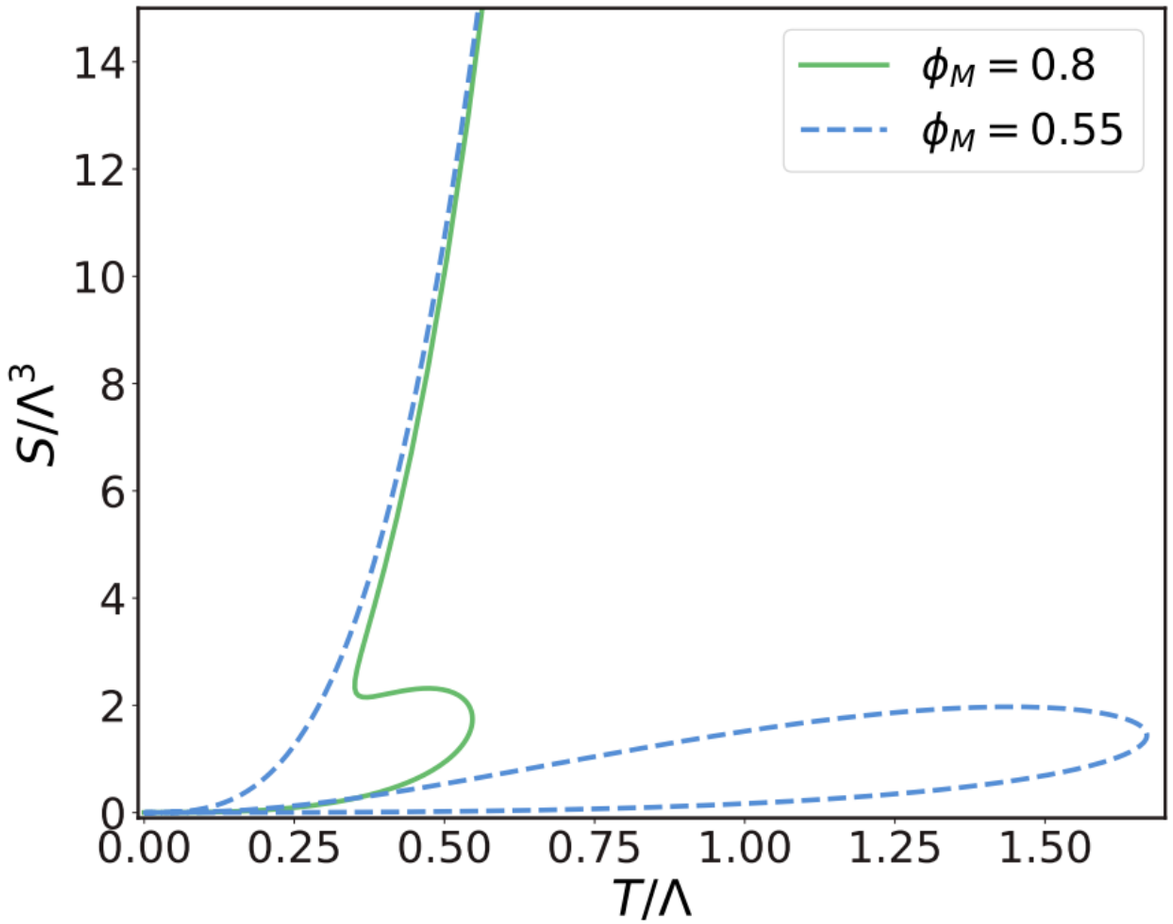


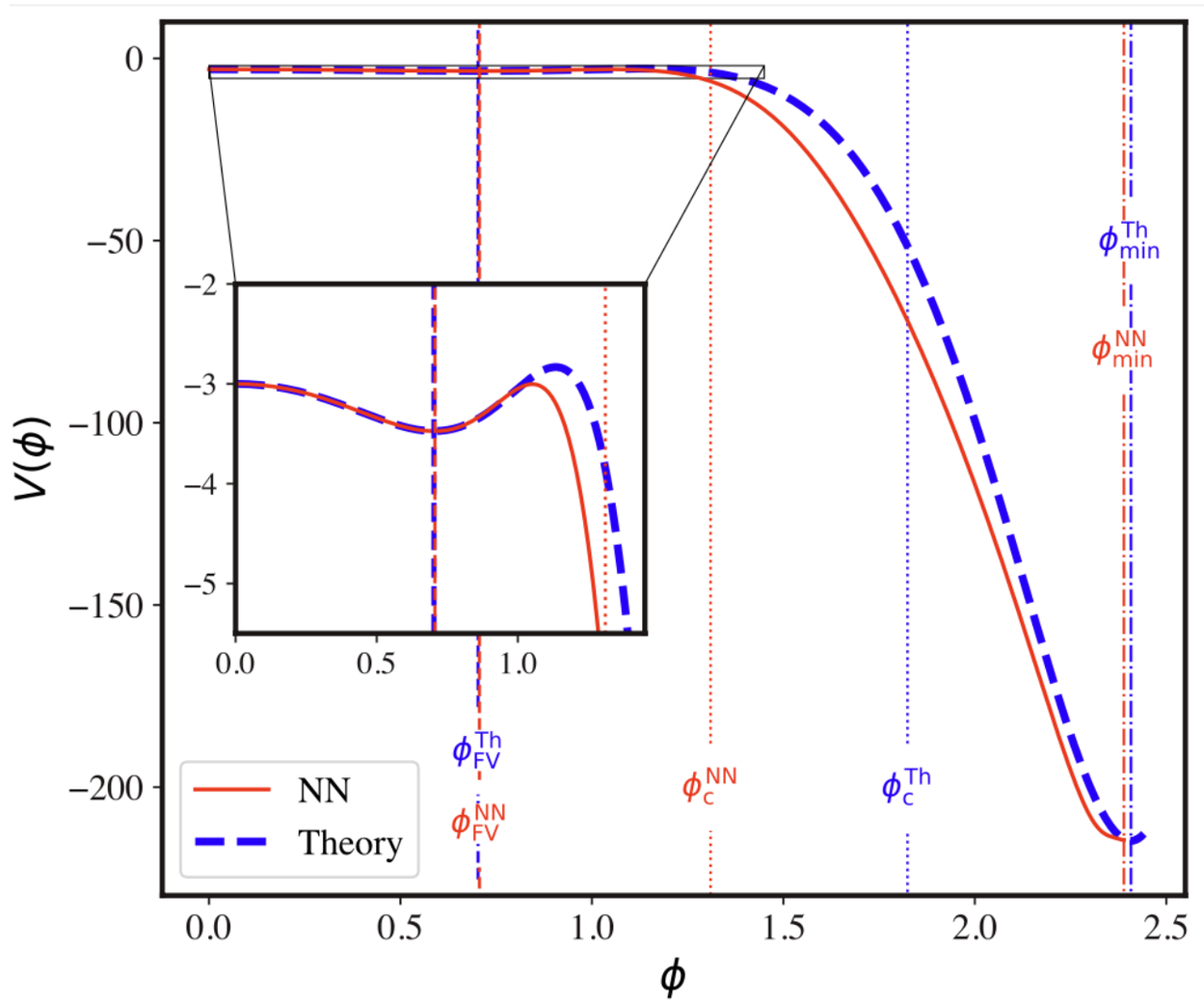


$V(\phi)$ recovered to **sub-percent** accuracy (rms < 0.5 %), S(T) to ≈ 1 %

Results: false vacua

Jiménez, Mateos, Protopapas, PSV, Tarancón-Álvarez, Tejerina-Pérez '26





Conclusions & future work

- **Motivation & Setup:** first-order transitions → bubbles → sound waves → GWs
  holography computes the whole chain from first principles once the gravity theory is known

- **PINNs:** reconstruct spacetime from the equation of state: crossover, 2nd- and 1st-order transitions to sub-percent accuracy (2403.14763) the strongest transitions (false vacua) now within reach (2606.30117)

- Future work:



  - Observational data: NICER (in the future, NS mergers such as GW170817)
  - PINNs latent space: efficient transfer learning for non-linear PDEs Solé-Vilaró et al. 26', under review (ICLR 2027)
  - Modelling against future signals: predict GW spectra and compare with data in Bayesian fit

谢谢大家！