

A Mesh-Free PINN Framework for Scalable Stellar Structure Modeling

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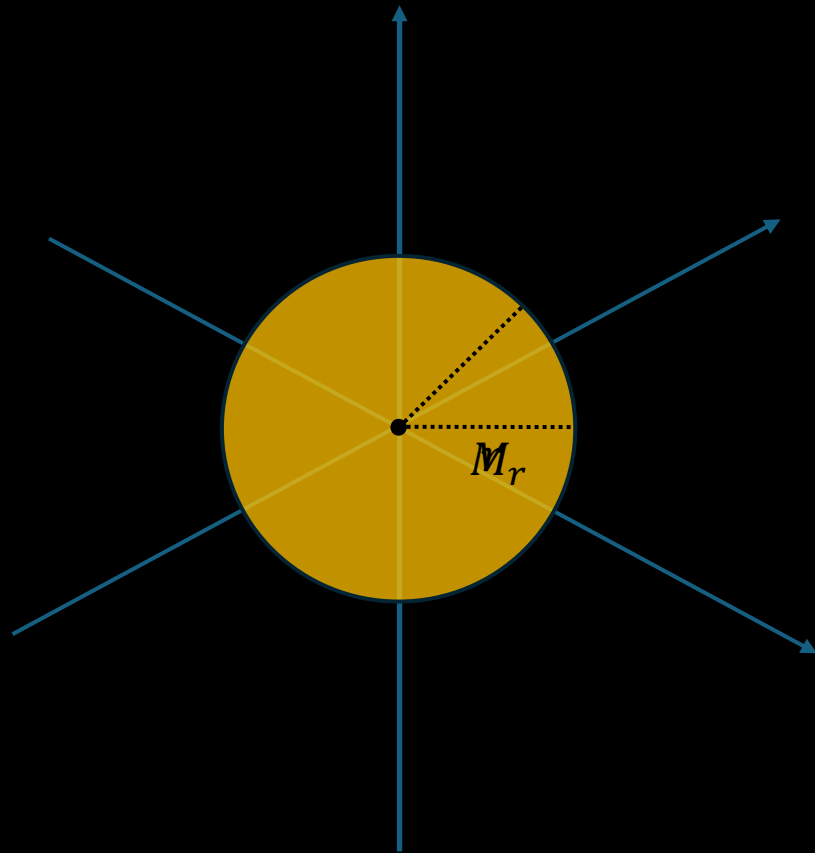
Work by: Manuel Ballester, Santiago Lopez-Tapia, Seth Gossage, Patrick Koller, Philipp M. Srivastava, Ugur Demir, Yongseok Jo, Almudena P. Marquez, Christoph Wuersch, Souvik Chakraborty, Vicky Kalogera, and Aggelos Katsaggelos

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Defining Stellar Structure



- Consider temperature varying from the star's center to its surface
- Assume temperature changes equally in all radial directions
- Instead of using r as a spatial coordinate, we consider the mass enclosed

Stellar Structure Quantities Auxiliary Quantities

Pressure – $P(M_r)$

Luminosity – $L_r(M_r)$

Radius – $r(M_r)$

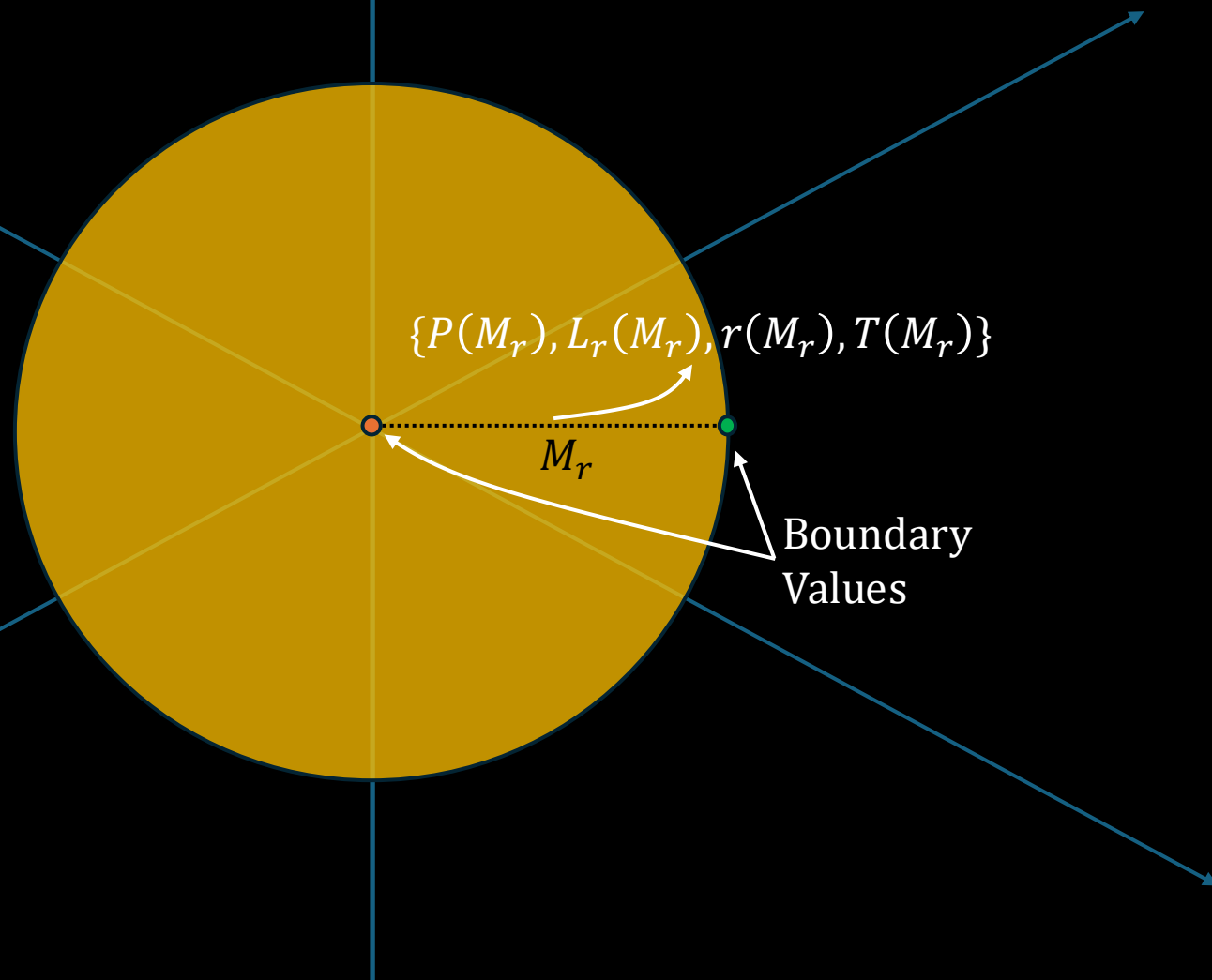
Temperature – $T(M_r)$

Density – $\rho(M_r)$

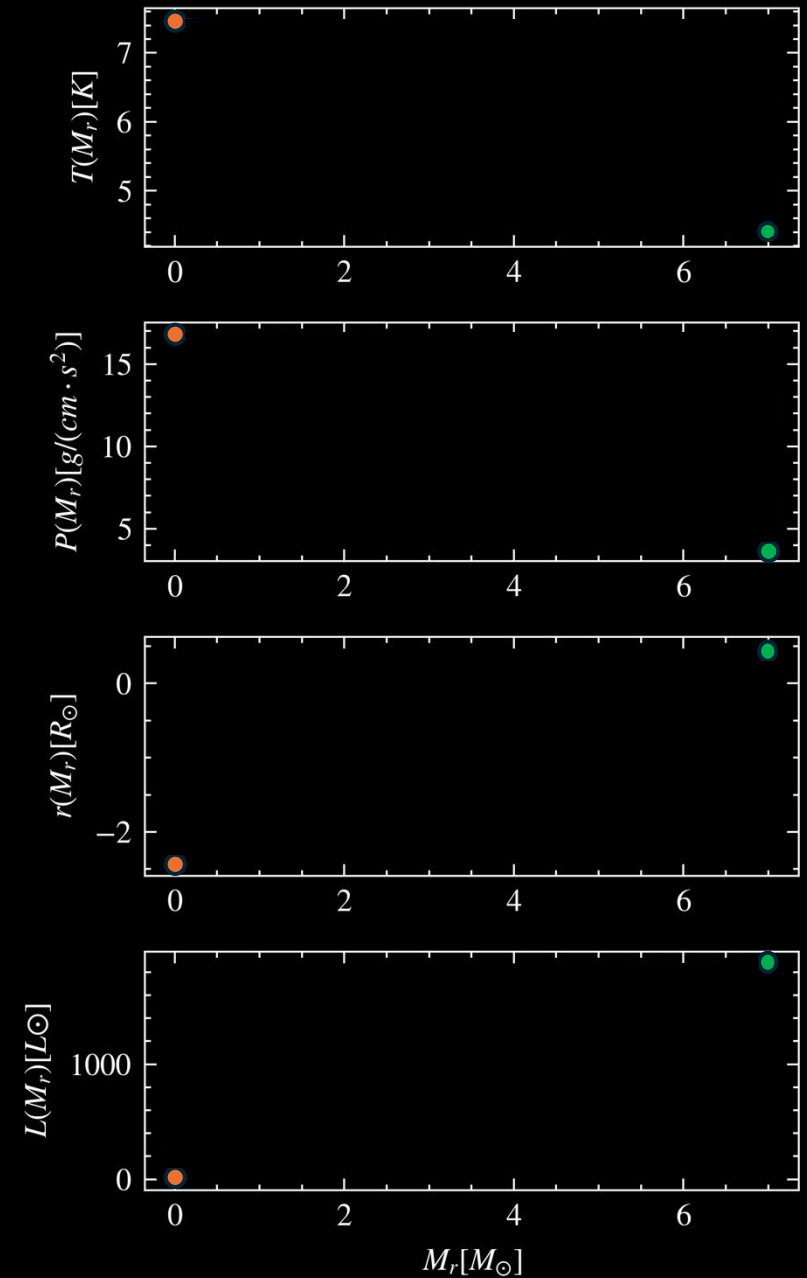
Opacity – $\kappa(M_r)$

Energy – $\epsilon(M_r)$

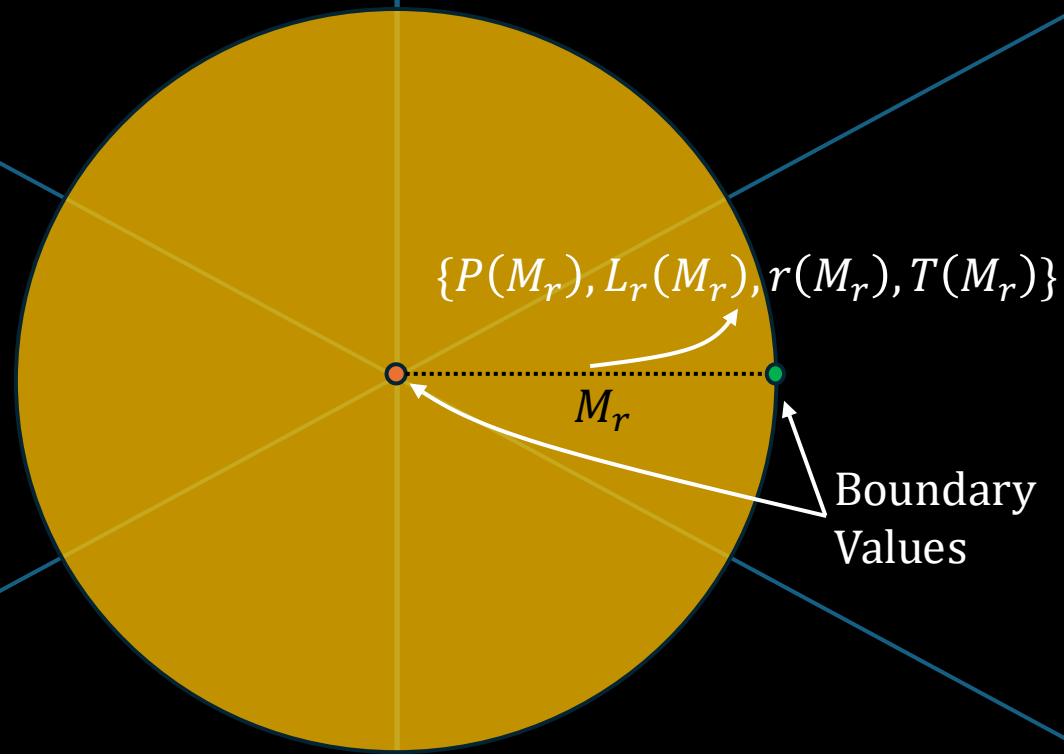
Problem Definition



Example Stellar Profile



Problem Definition

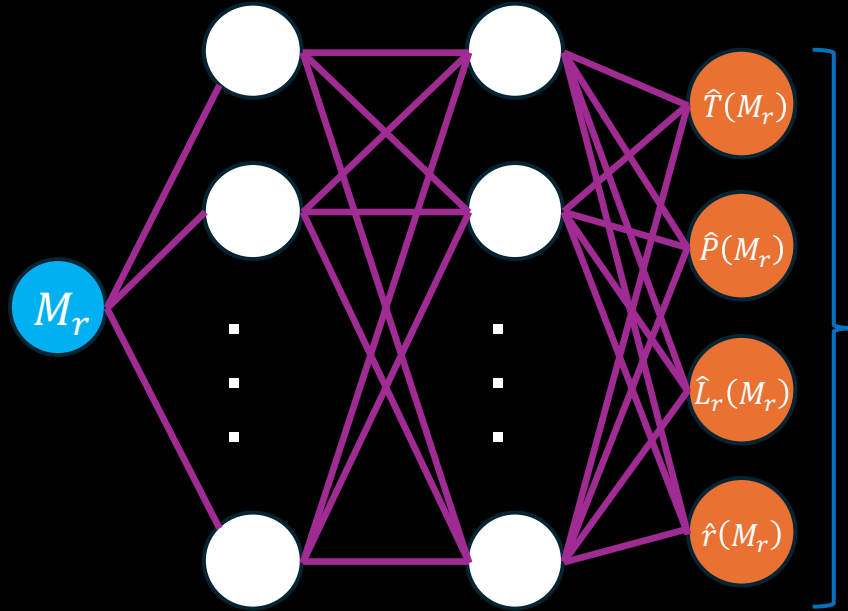


MESA

- Traditionally solved using stellar structure equations and finite difference
- Stellar structure equations are stiff and highly non-linear
- A single simulation can take many hours
- What if we can accelerate this?

(Paxton et al. 2011–2019; Jermyn et al. 2023)

A neural network for stellar structure



Multi-layer Perceptron (MLP)

$$f_{\theta}(M_r)$$

Traditionally Trained
Using a Loss Function
with gradient descent

$$\begin{aligned} & \left(\hat{T}(M_r) - T(M_r) \right)^2 \\ & + \\ & \left(\hat{P}(M_r) - P(M_r) \right)^2 \\ & + \\ & \left(\hat{L}_r(M_r) - L_r(M_r) \right)^2 \\ & + \\ & \left(\hat{\rho}(M_r) - \rho(M_r) \right)^2 \end{aligned}$$

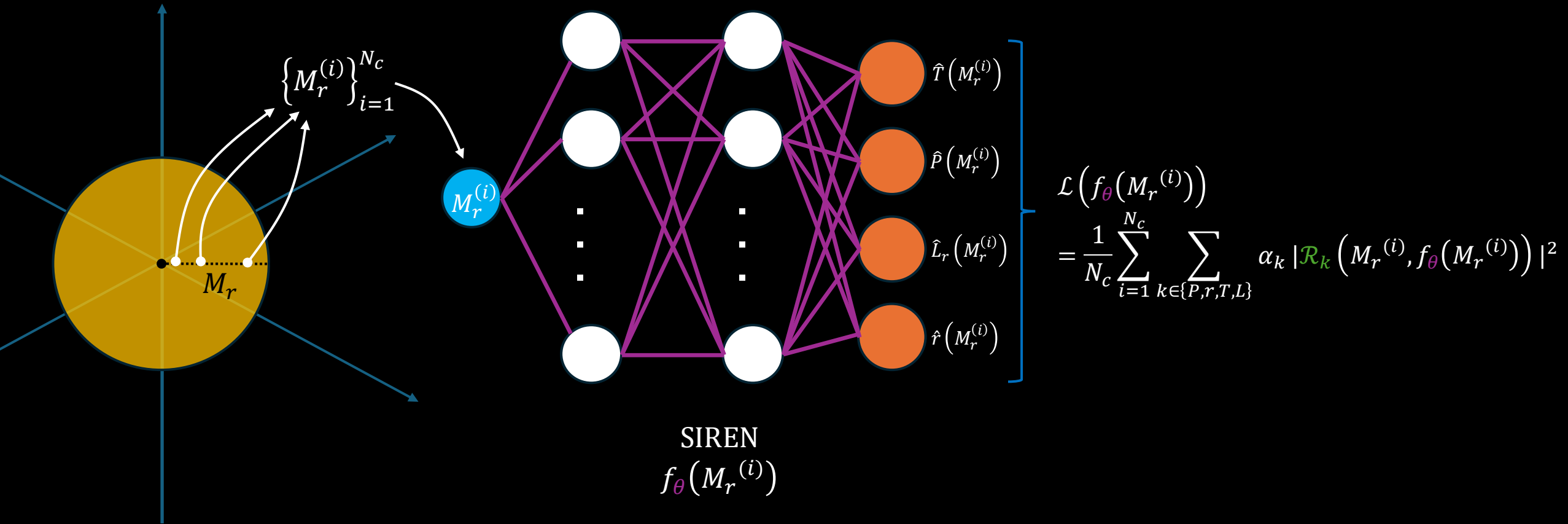
Minimize

What if we have no
data?

Stellar Structure Equations as a Loss Function

$$\begin{array}{ll}
 (1) \quad \frac{\partial P}{\partial M_r} = -\frac{\beta_a M_r}{r^4} & \mathcal{R}_P = \frac{\partial \hat{P}}{\partial M_r} + \frac{\beta_a M_r}{\hat{r}^4} \\
 (2) \quad \frac{\partial r}{\partial M_r} = \frac{\beta_b}{r^2 \rho} & \mathcal{R}_r = \frac{\partial \hat{r}}{\partial M_r} - \frac{\beta_b}{\hat{r}^2 \rho} \\
 (3) \quad \frac{\partial T}{\partial M_r} = -\frac{\beta_c L_r}{r^4} \nabla(M_r, \kappa) & \mathcal{R}_T = \frac{\partial \hat{T}}{\partial M_r} + \frac{\beta_c \hat{L}_r}{\hat{r}^4} \nabla(M_r, \kappa) \\
 (4) \quad \frac{\partial L_r}{\partial M_r} = \beta_d \epsilon & \mathcal{R}_{L_r} = \frac{\partial \hat{L}_r}{\partial M_r} - \beta_d \epsilon
 \end{array}
 \left. \vphantom{\begin{array}{l} \mathcal{R}_P \\ \mathcal{R}_r \\ \mathcal{R}_T \\ \mathcal{R}_{L_r} \end{array}} \right\} \text{Quantities to Minimize}$$

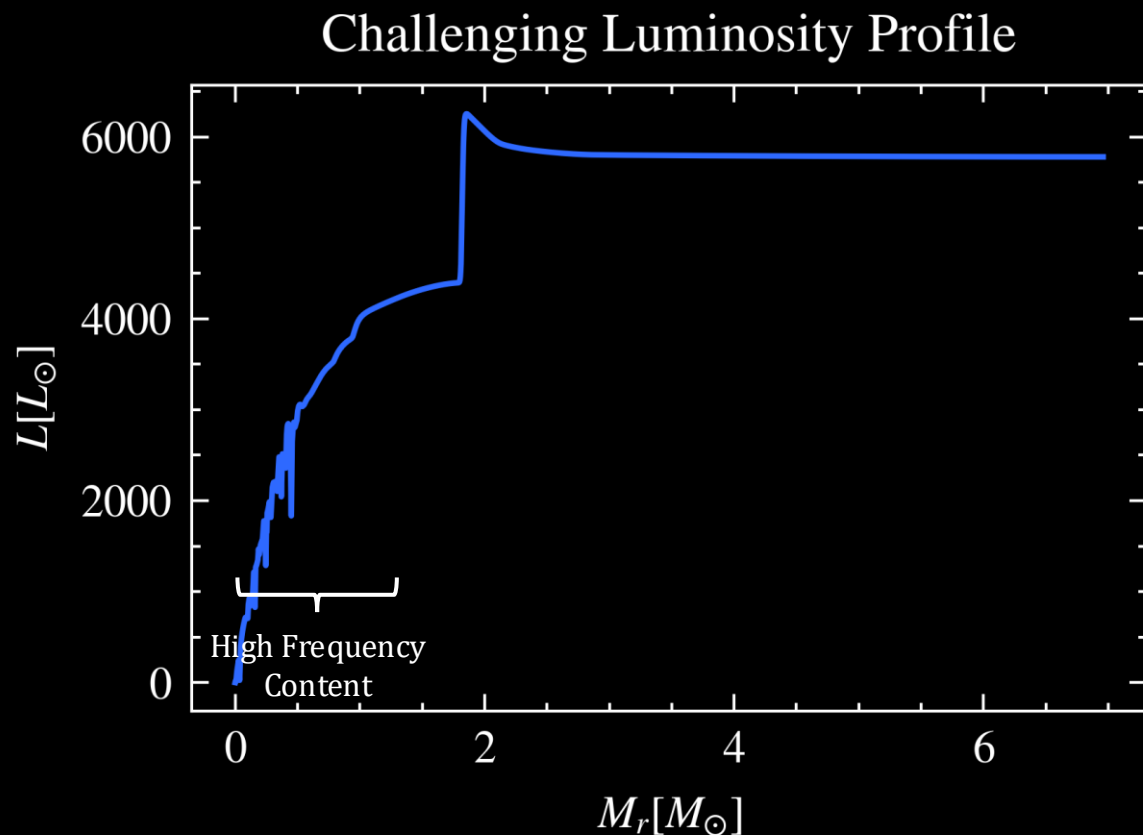
PINNs for stellar structure



SIREN
 $f_\theta(M_r^{(i)})$

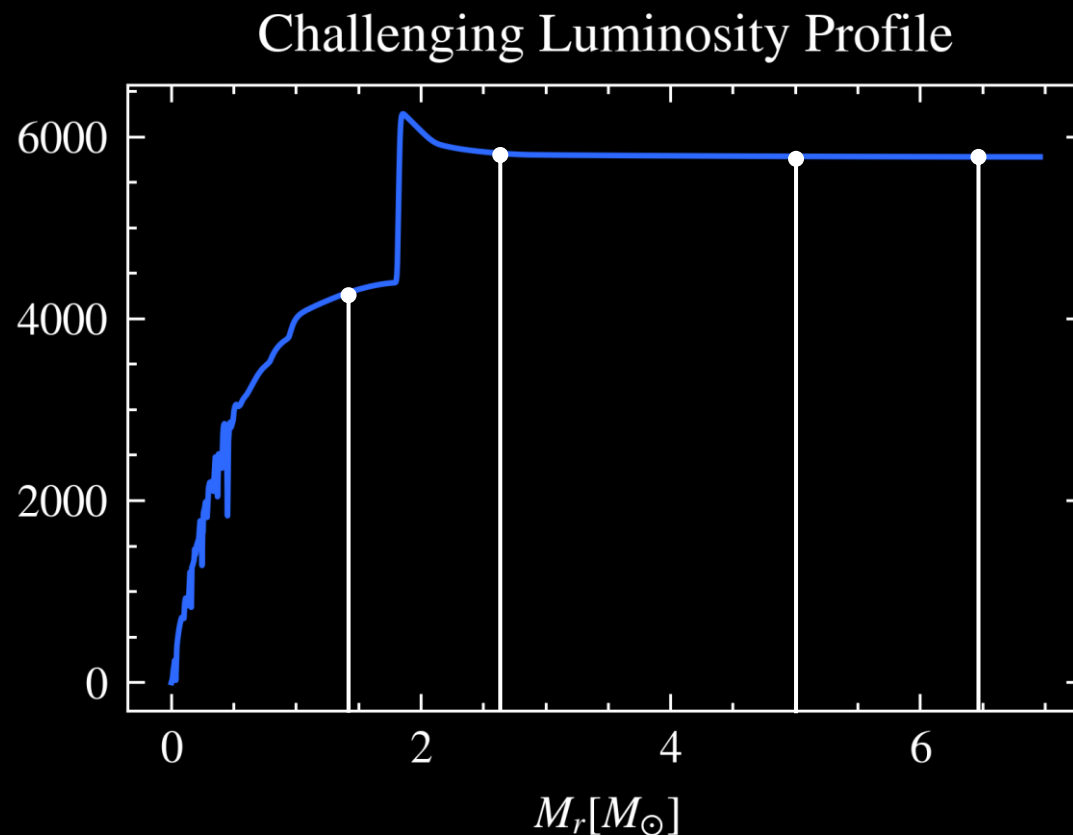
Challenges with PINNs

Spectral bias



A. Rahimi and B. Recht, "Random features for large-scale kernel machines," in *Advances in Neural Information Processing Systems 20 (NIPS 2007)*, J. Platt, D. Koller, Y. Singer, and S. Roweis, Eds. Curran Associates, Inc., 2007.

Collocation point selection



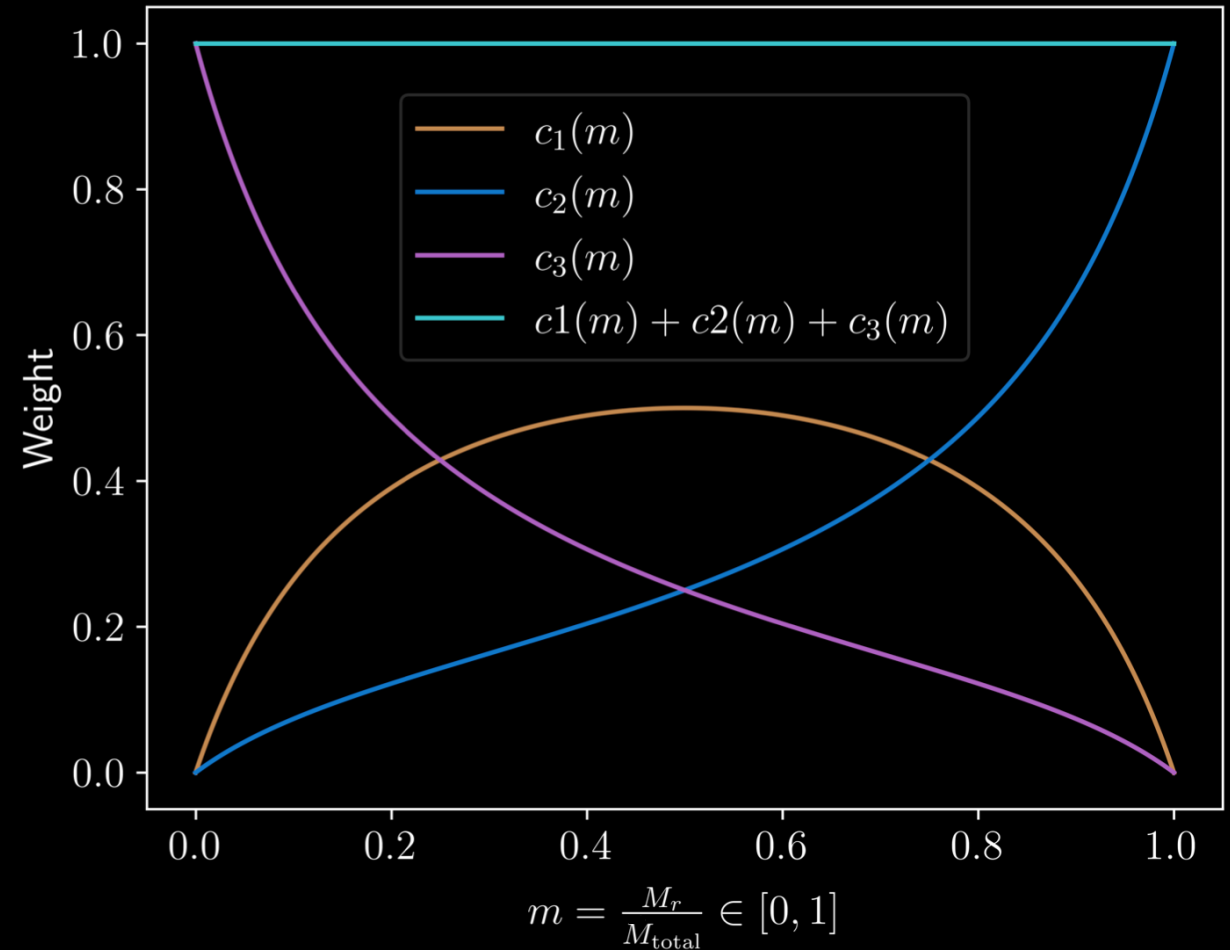
S. J. Anagnostopoulos, J. D. Toscano, N. Stergiopoulos, and G. E. Karniadakis, "Residual-based attention and connection to information bottleneck theory in PINNs," arXiv preprint arXiv:2307.00379, 2023.

Boundary Conditions

- $f_{\theta}(M_r^{(i)})$ is unconstrained and can give values outside of known boundary conditions
- We constraint the output of each variable using the following function:

$$g_{\theta}(m) = c_1(m)f_{\theta}(M_r) + c_2(m)BC(M_r) + c_3(m)BC(0), \quad m = \frac{M_r}{M_{total}}$$

- This enforces a hard constraint to the output of the system at the boundaries



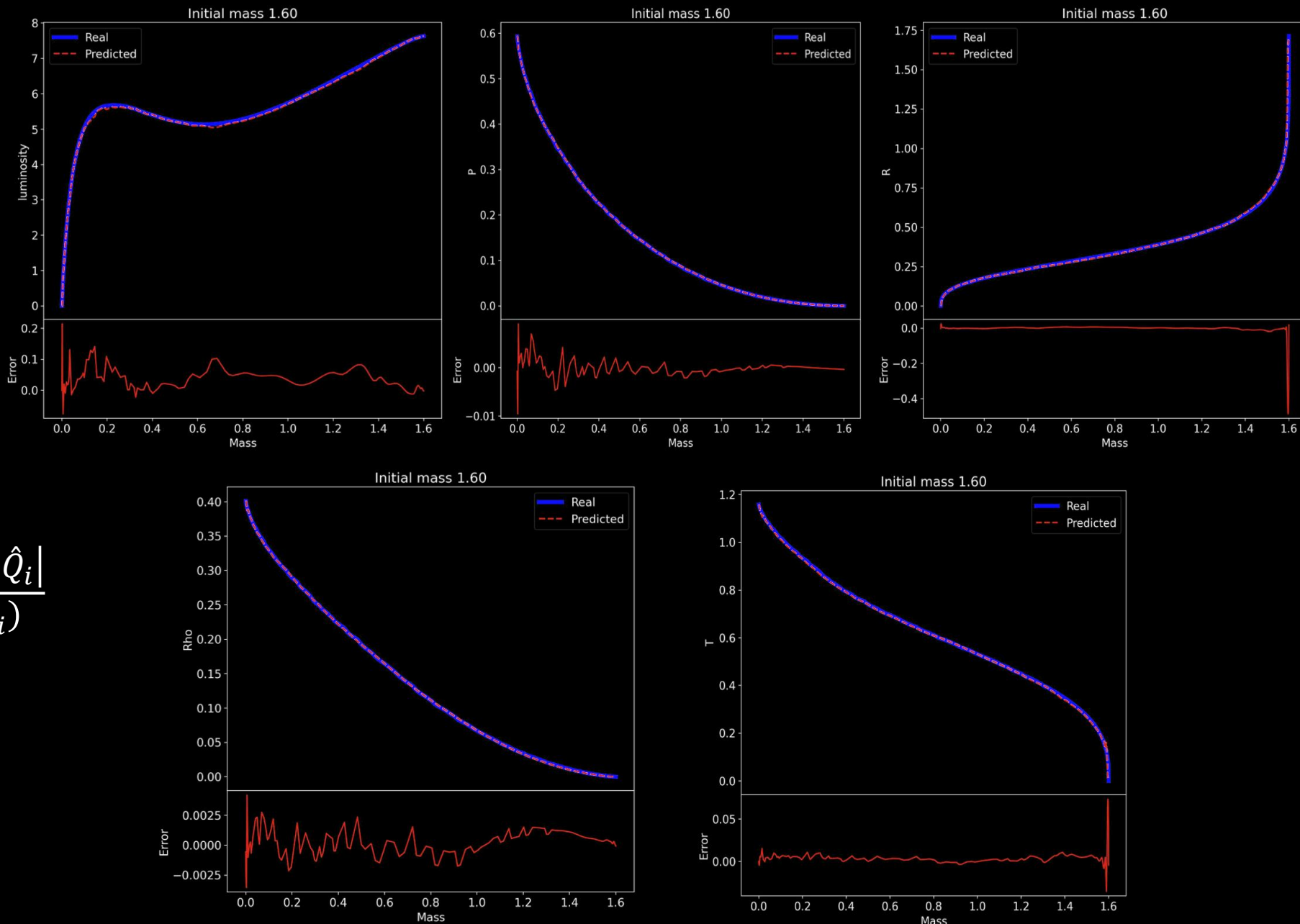
Results

Tested over a range
of $M_T = 0.4M_\odot$ to
 $M_T = 9.9M_\odot$

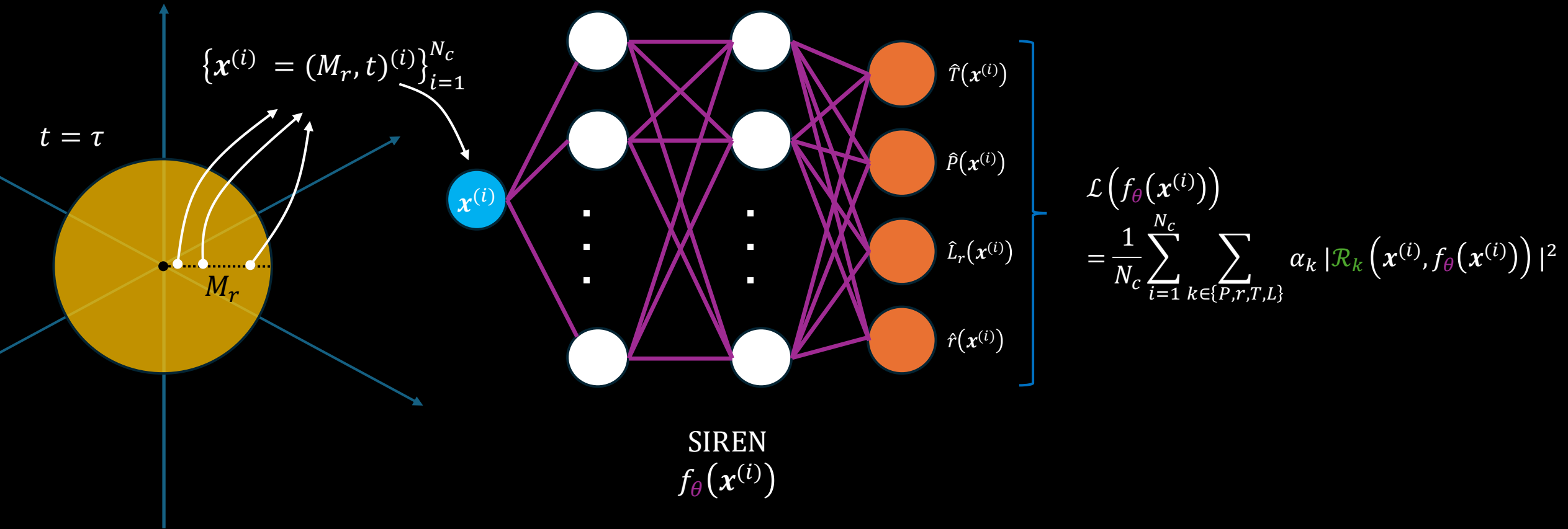
$$R^2 = 99.98\%$$

Average MRAE of 3.06%

$$MRAE(Q, \hat{Q}) = \frac{1}{N} \sum_{i=1}^N \frac{|Q_i - \hat{Q}_i|}{\sigma(Q_i)}$$

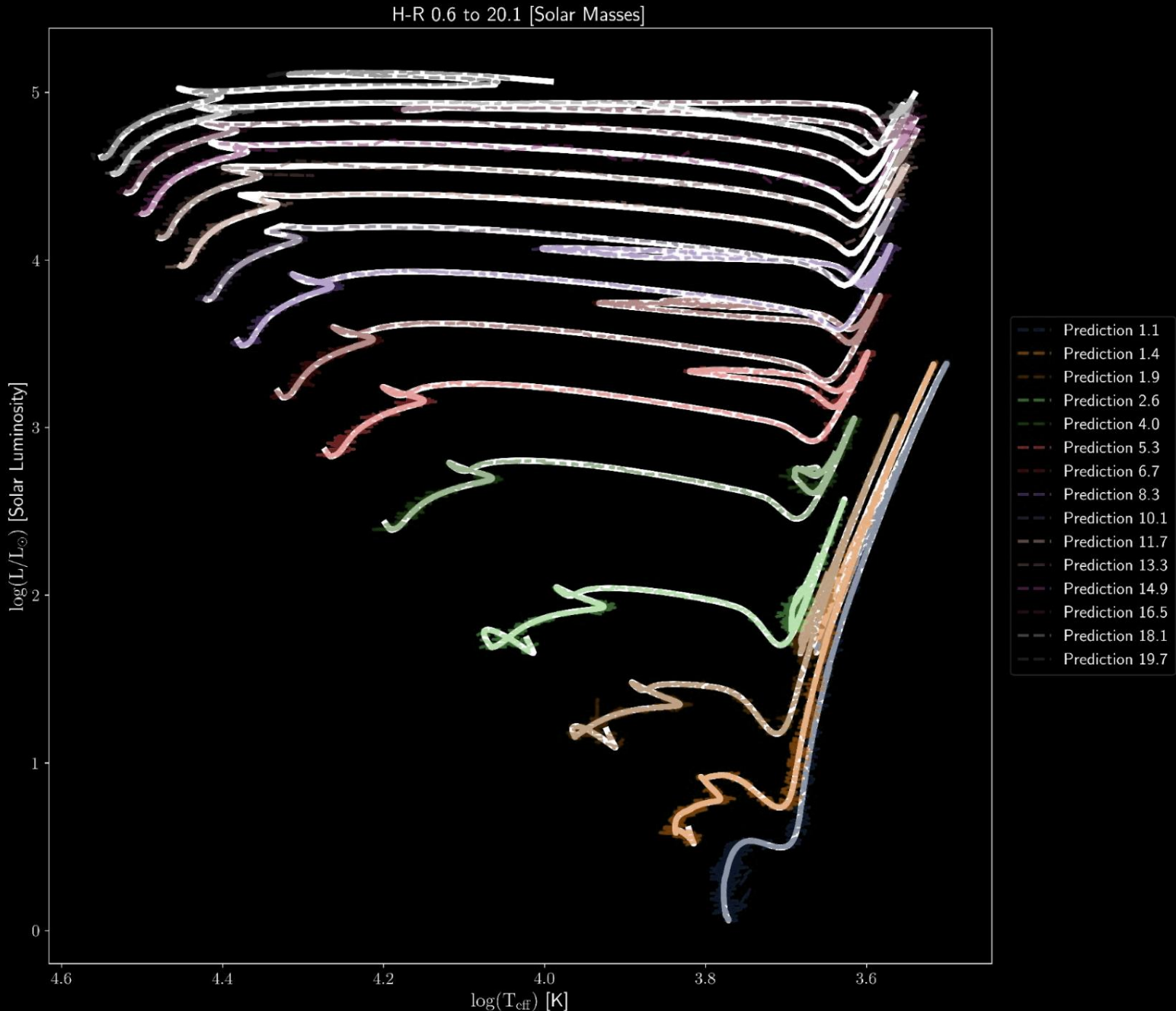


PINNs for stellar structure evolution



Results

- We utilize key advancements in the scientific machine learning literature enabling a PINN to be used as a solver for stiff, non-linear equations
- This paves the way to generalizing this system to be able to consider many boundaries with one system
- This work builds the foundation for accelerating stellar structure evolution simulation for both single and binary stars



Ongoing and Future Work

Stellar Structure

- Prediction of ϵ using an auxiliary neural network, rendering the presented PINN “MESA-Free”
- Physics Informed Neural Spline Architecture (PINSA) – Total Mass is given as additional input and generalizes to stellar structures within a trained mass range

Stellar Structure Evolution

- A hybrid approach which solves for stellar structure using a physics informed neural operator (PINO), but utilizes finite difference for computing change in composition
- Neural operator inspired methods for quantity predictions of binary star systems

Looking Forward to Your Questions!



Philipp M.
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Manuel Ballester



Santiago Lopez-
Tapia



Seth Gossage



Patrick Koller



Ugur Demir



arXiv Paper



Aggelos
Katsaggelos



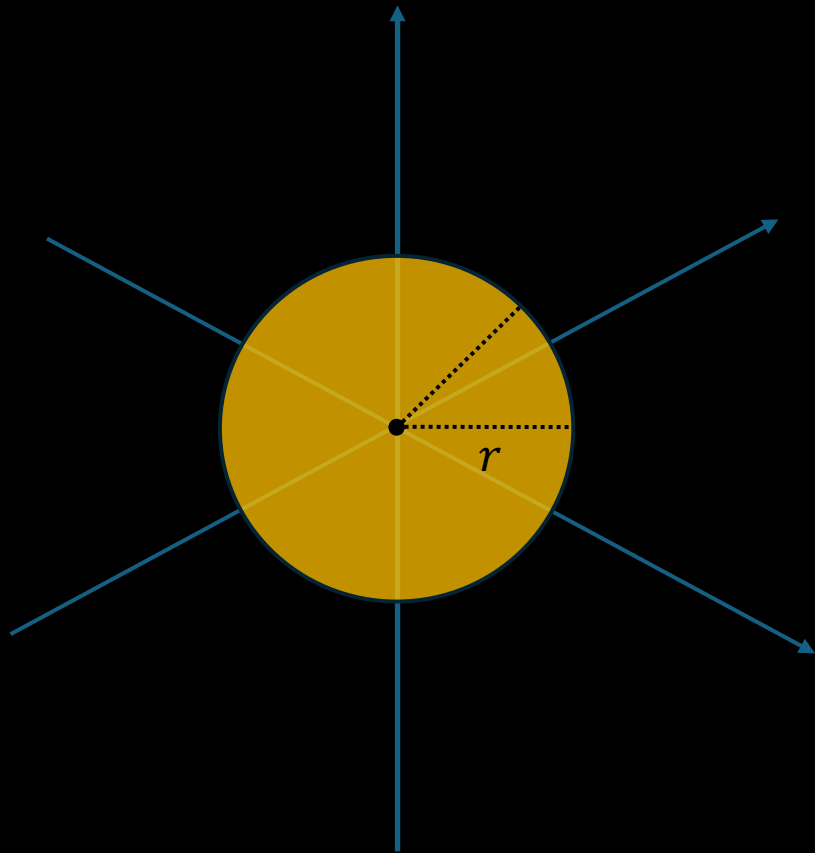
Vicky Kalogera

Backup Slides

Implementation Details

- Auxiliary networks utilize Random Fourier Features [1] and sinusoidal activations [2]
- PINN uses only sinusoidal activations
- Trained for 10,000 with a batch size of 256 with AdaM [3] optimizer with a scaling factor for $\lambda = 5 \times 10^{-2}$
- SP-PINN [4] is used to accelerate gradient computation
- Mass range is $M_T = 0.4M_\odot$ to $M_T = 9.9M_\odot$ using 96 uniformly spaced samples per profile

Defining Stellar Structure



- Consider temperature varying from the star's center to its surface
- We assume that temperature varying from the center to any point on the surface is the same (spherical symmetry)
- Consider other quantities of interest

Stellar Structure Quantities

Pressure - $P(r)$

Luminosity - $L_r(r)$

Mass - $M_r(r)$

Temperature - $T(r)$

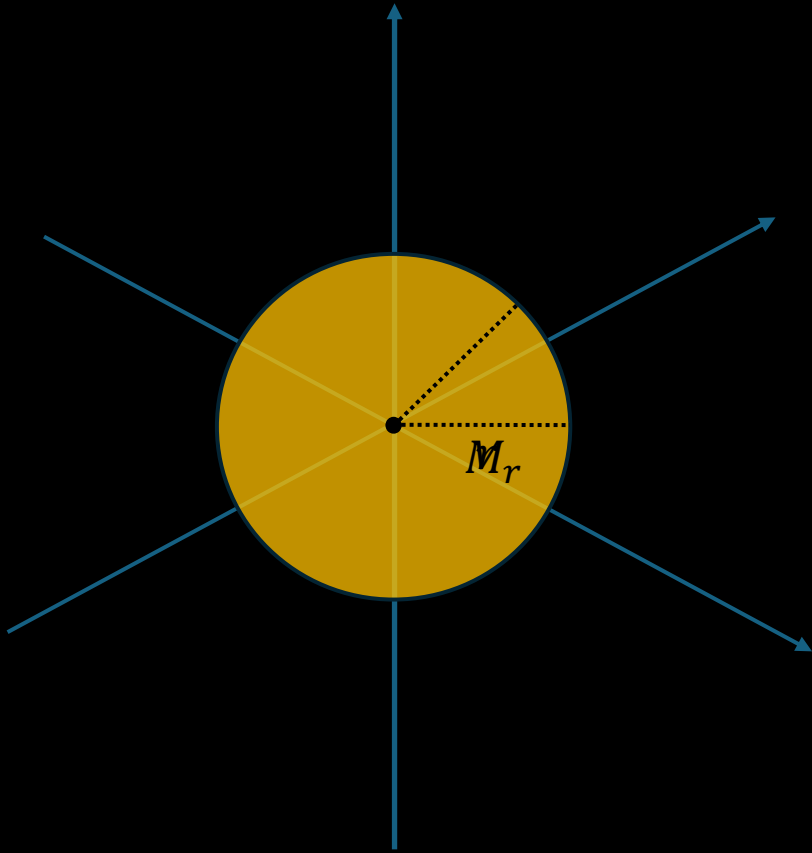
Auxiliary Quantities

Density - $\rho(r)$

Opacity - $\kappa(r)$

Energy - $\epsilon(r)$

Change of Independent Variables



- Instead of using radius r as a spatial coordinate, we can consider the mass enclosed at r as the spatial coordinate
- We denote the mass enclosed at a given radius as M_r
- This can be done because M_r is monotonically increasing with r

<u>Stellar Structure Quantities</u>	<u>Auxiliary Quantities</u>
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Pressure – $P(M_r)$

Density – $\rho(M_r)$

Luminosity – $L_r(M_r)$

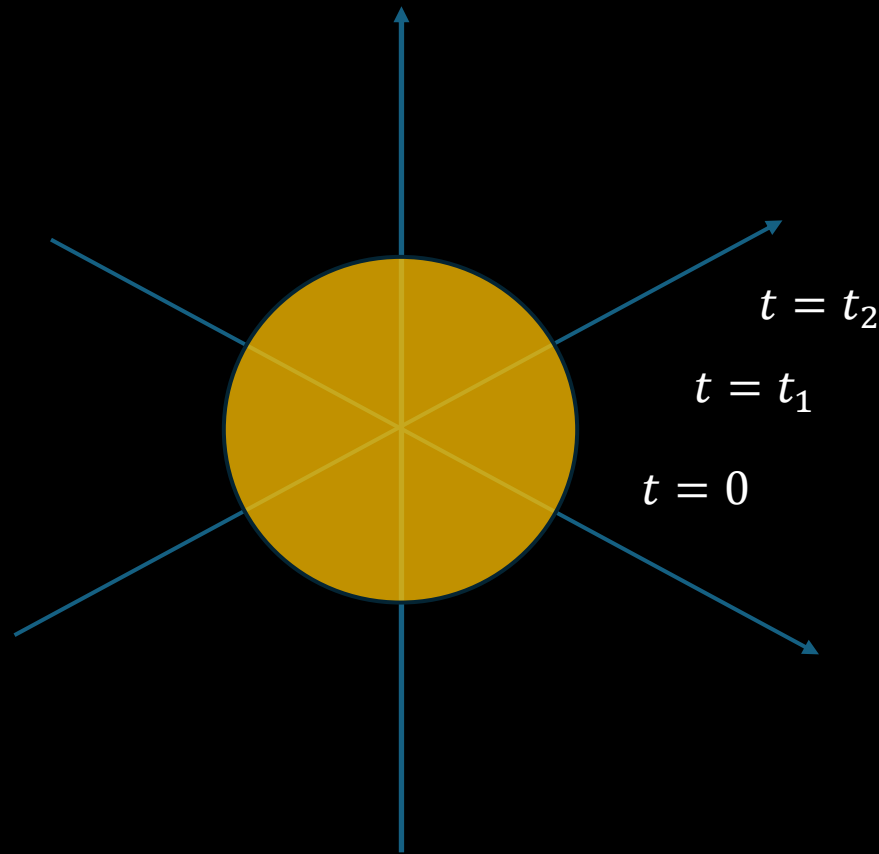
Opacity – $\kappa(M_r)$

Radius – $r(M_r)$

Energy – $\epsilon(M_r)$

Temperature – $T(M_r)$

Stellar Structure Evolution



Stellar Structure Quantities

Pressure – $P(M_r, t)$

Luminosity – $L_r(M_r, t)$

Radius – $r(M_r, t)$,

Temperature – $T(M_r, t)$

Auxiliary Quantities

Density – $\rho(M_r, t)$

Opacity – $\kappa(M_r, t)$

Energy – $\epsilon(M_r, t)$

Stellar Structure

(in Hydrostatic and Thermal Equilibrium)

Where,

$$(1) \frac{\partial P}{\partial M_r} = \frac{\beta_a M_r}{r^4}$$

$$\nabla_{ad} = \frac{d \ln T}{d \ln P}$$

$$(2) \frac{\partial r}{\partial M_r} = \frac{\beta_b}{r^2 \rho}$$

$$(3) \frac{\partial T}{\partial M_r} = -\frac{\beta_c L_r}{r^4} \nabla(M_r, \kappa)$$

$$\nabla_{rad} = \frac{3\kappa P L_r}{16\pi a c G M_r T^4}$$

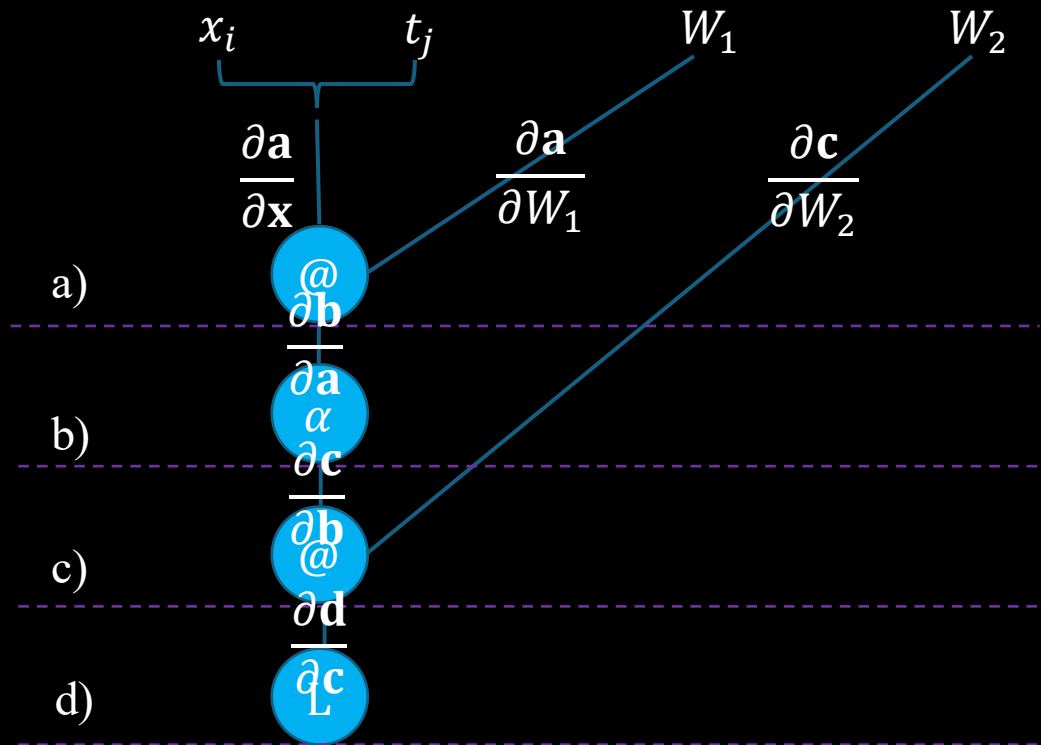
$$(4) \frac{\partial L_r}{\partial M_r} = \beta_d \epsilon$$

and

$$\nabla(M_r, \kappa) = \begin{cases} \nabla_{rad}, & \text{if } \nabla_{rad} \leq \nabla_{ad} \\ \nabla_{conv}, & \text{if } \nabla_{rad} > \nabla_{ad} \end{cases}$$

How can we enforce PDE residual?

Let $f_\theta(\cdot)$ be a two-layer neural network defined as $f_\theta(\mathbf{x}) = \alpha(\mathbf{x}W_1)W_2$ where $\theta = \{W_1, W_2\}$, $W_1 \in \mathbb{R}^{(2 \times d)}$, and $W_2 \in \mathbb{R}^{(d \times 1)}$



- Computational graph is built to compute gradients by default in many libraries
- This makes computing gradients with respect to the input easy
- However, it can be expensive, especially for higher-order derivatives
- Once computed we can enforce it easily in the loss function