Physics-Aware Recurrent Convolutions (PARC)

Stephen Baek

Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Physics-informed loss (Raissi et al.)

$$\partial_t u - \mathcal{N}(u) = 0$$

Recap of PINN and Neural Operator from a Differential Geometry Point of View

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$$\partial_t u - \alpha \nabla^2 u = 0$$

Heat equation

Recap of PINN and Neural Operator from a Differential Geometry Point of View

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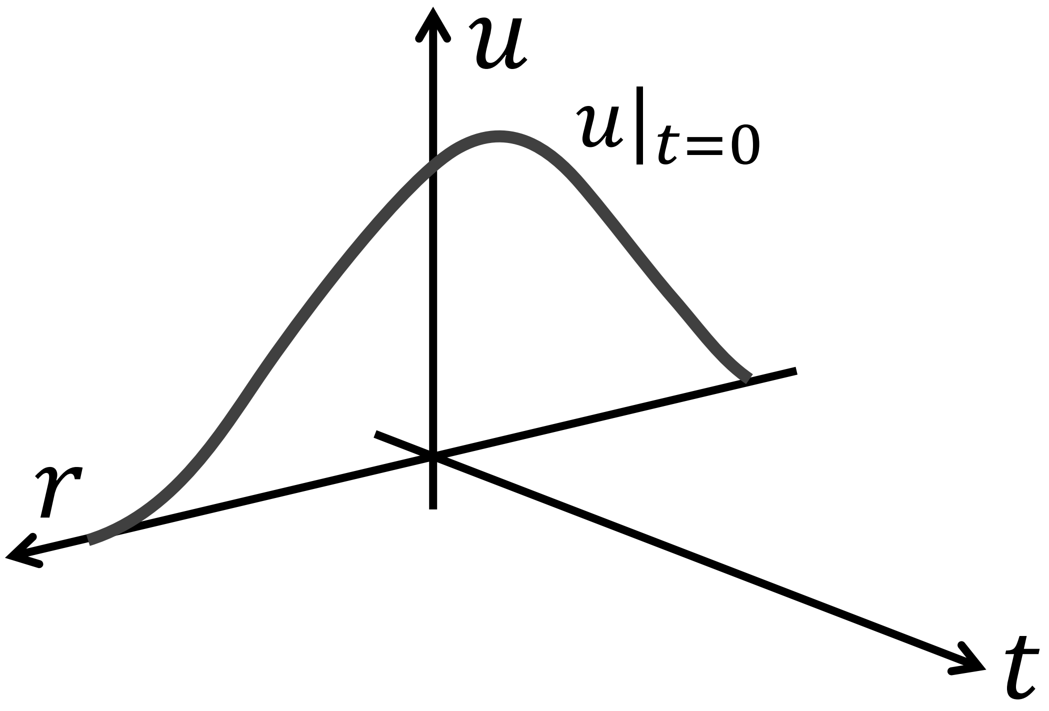

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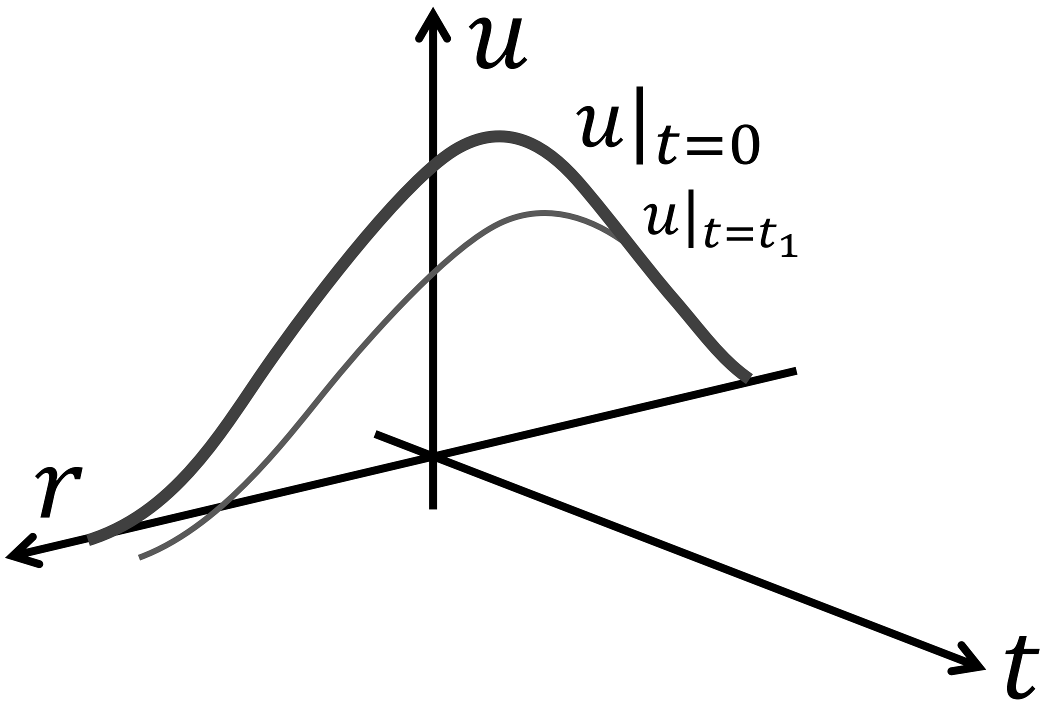

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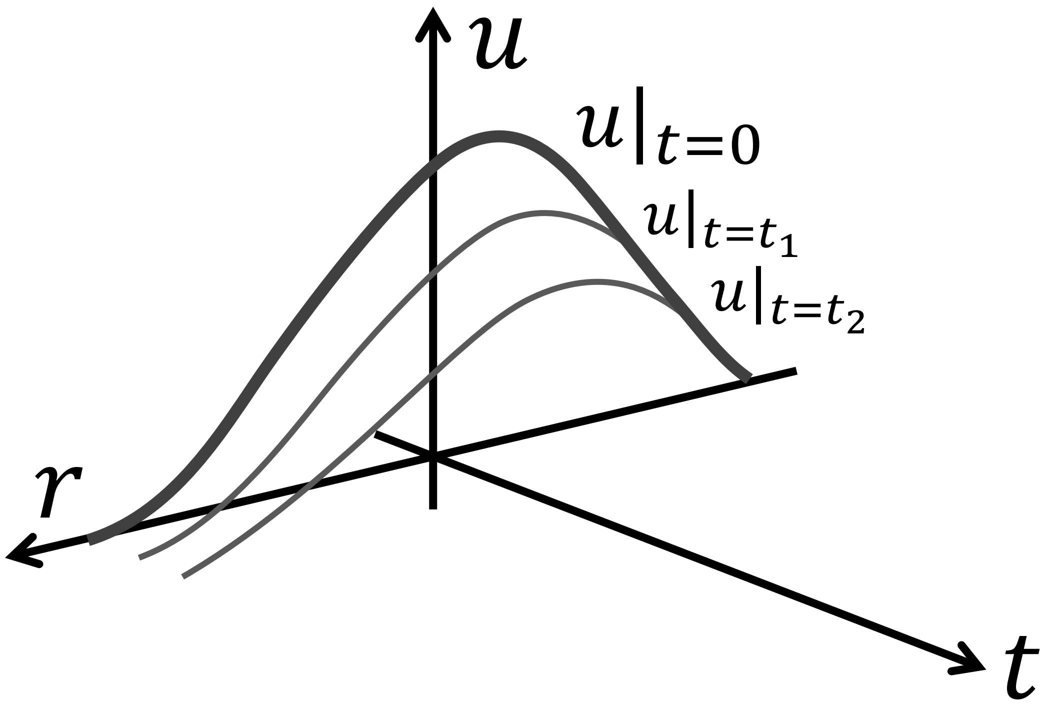

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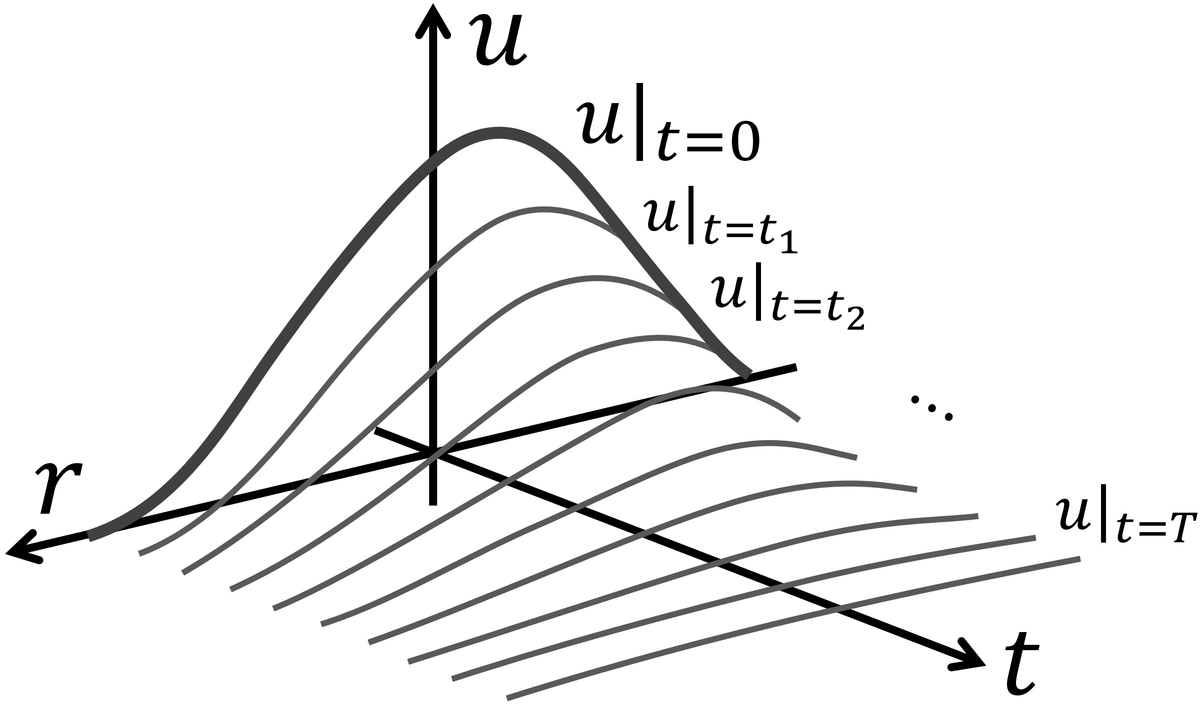

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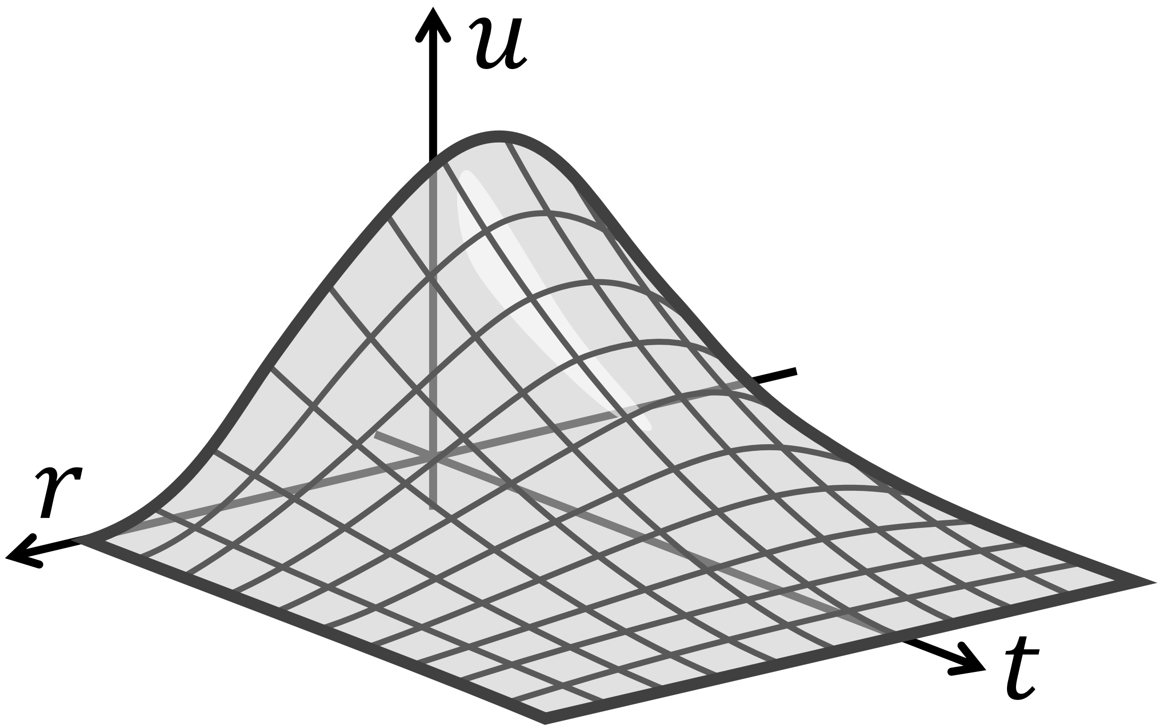

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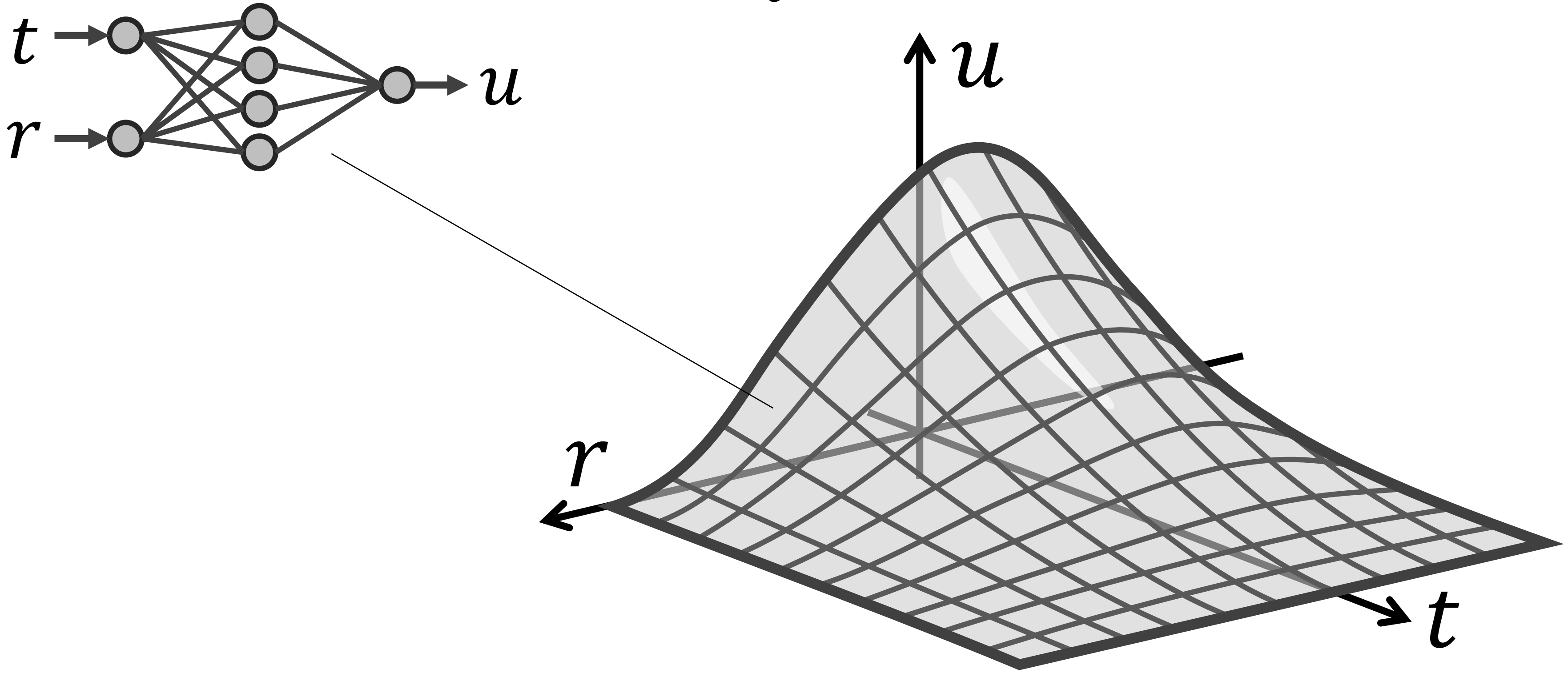

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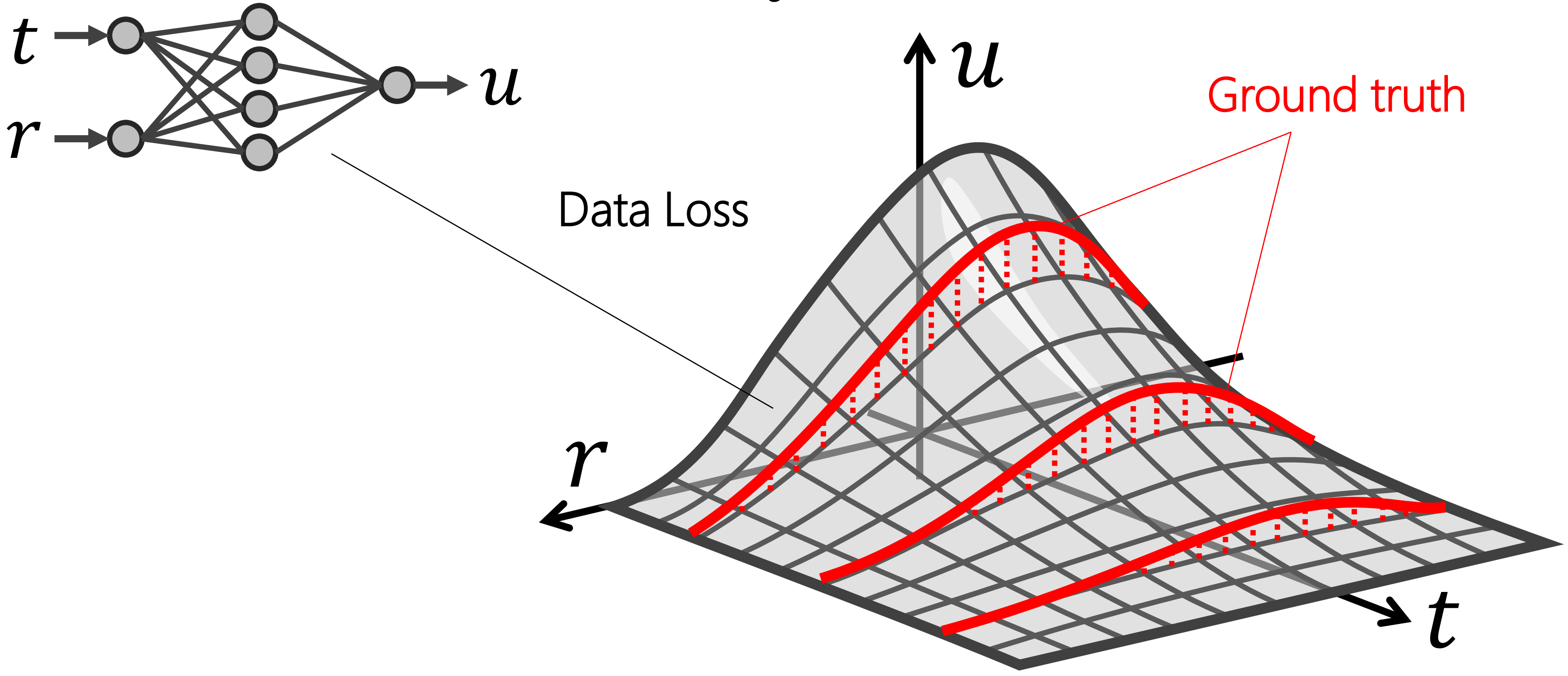

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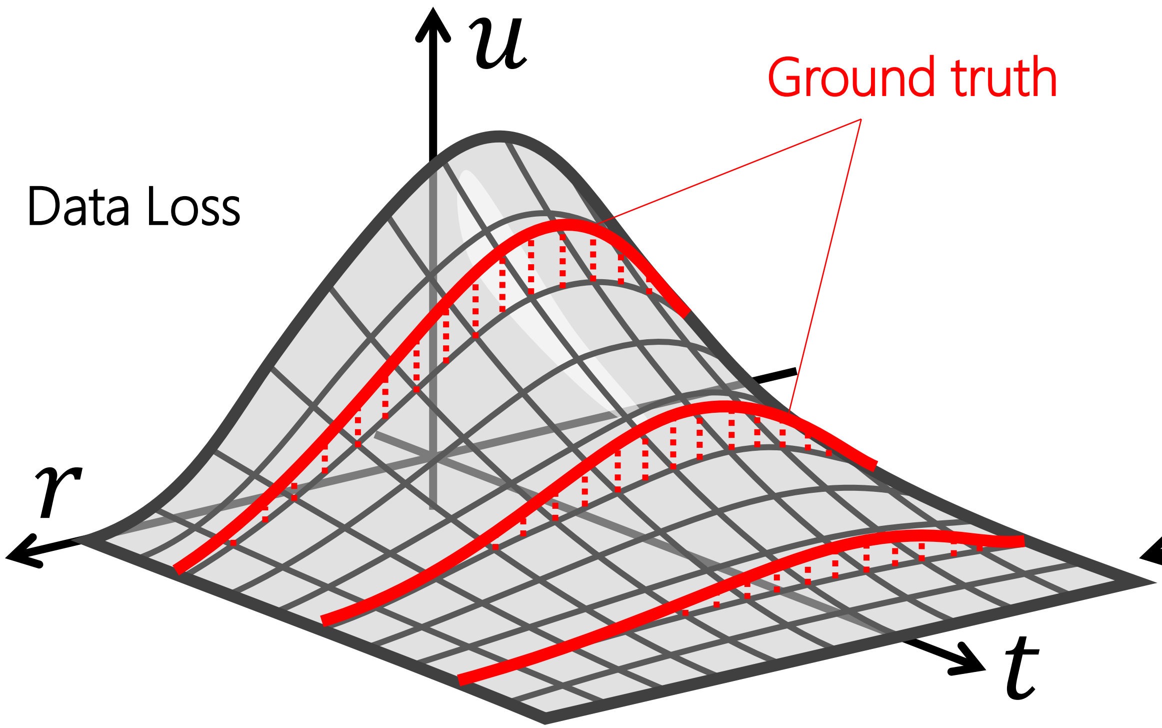
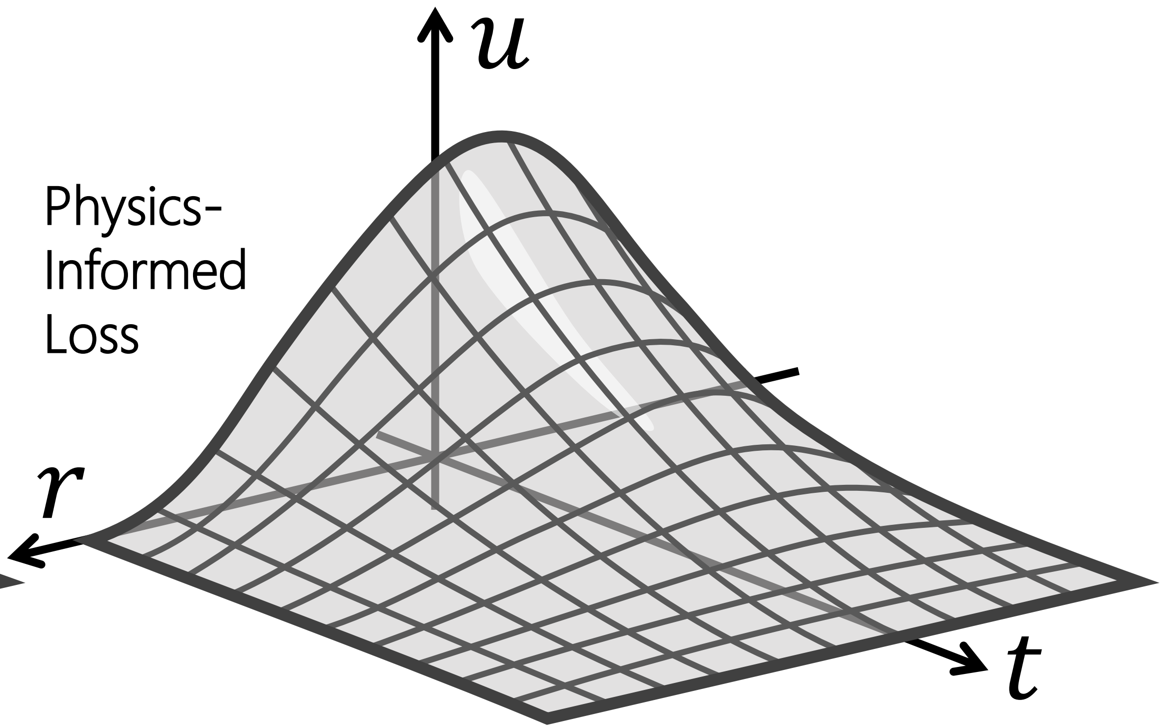
Data Loss



Physics-Informed Loss



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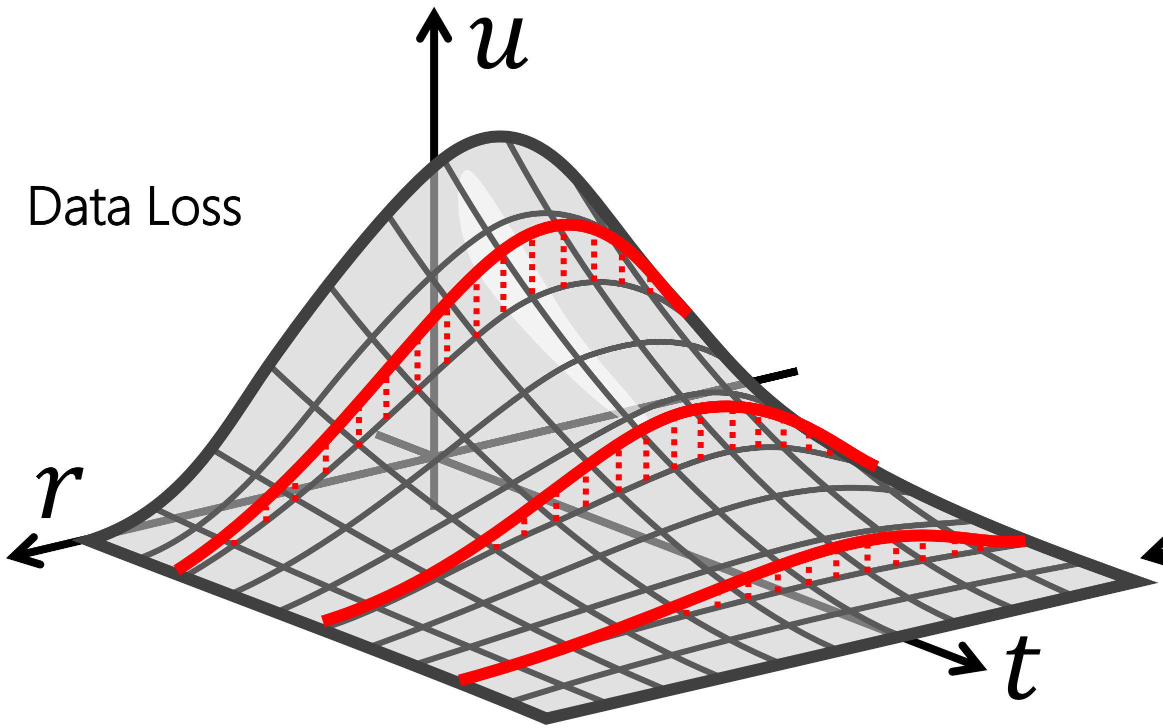
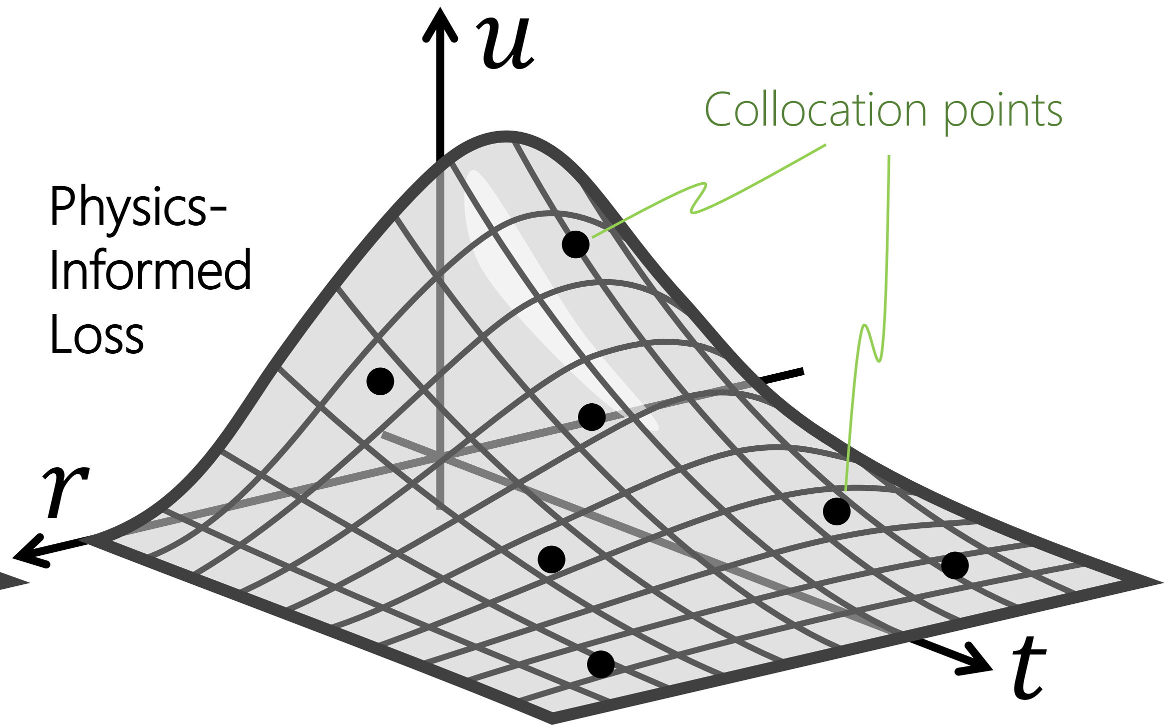


Physics-Informed Loss



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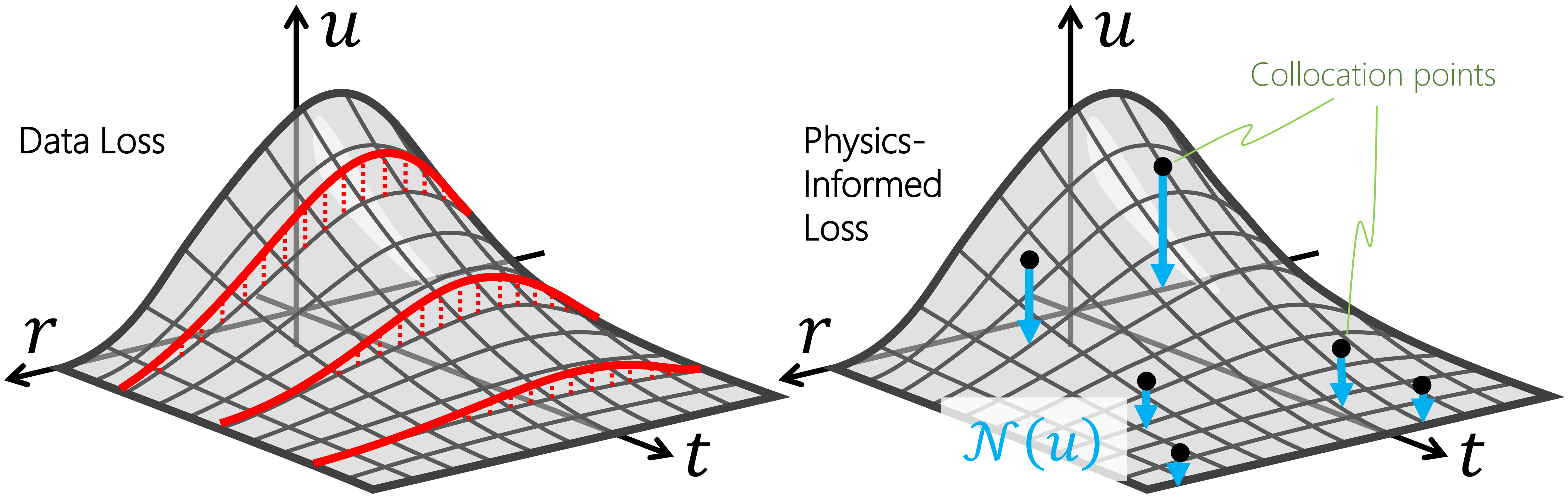

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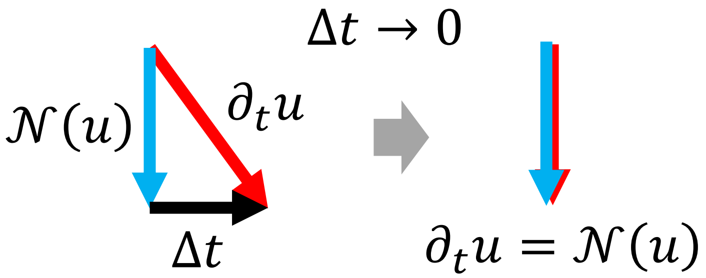

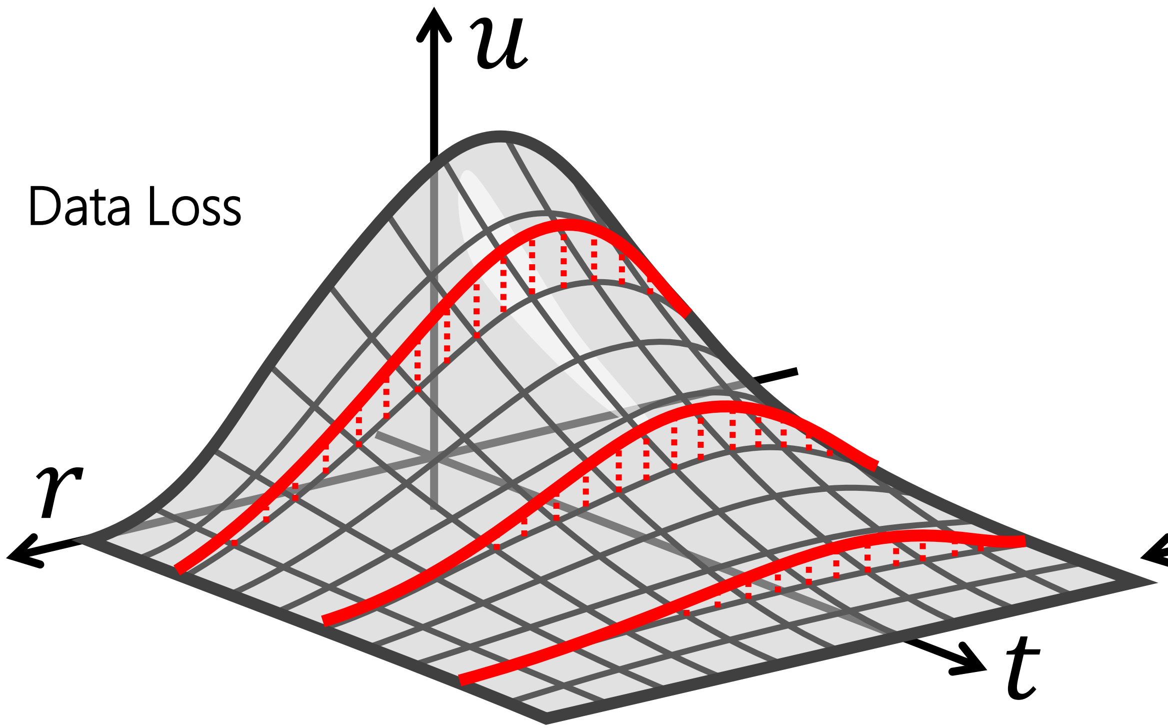

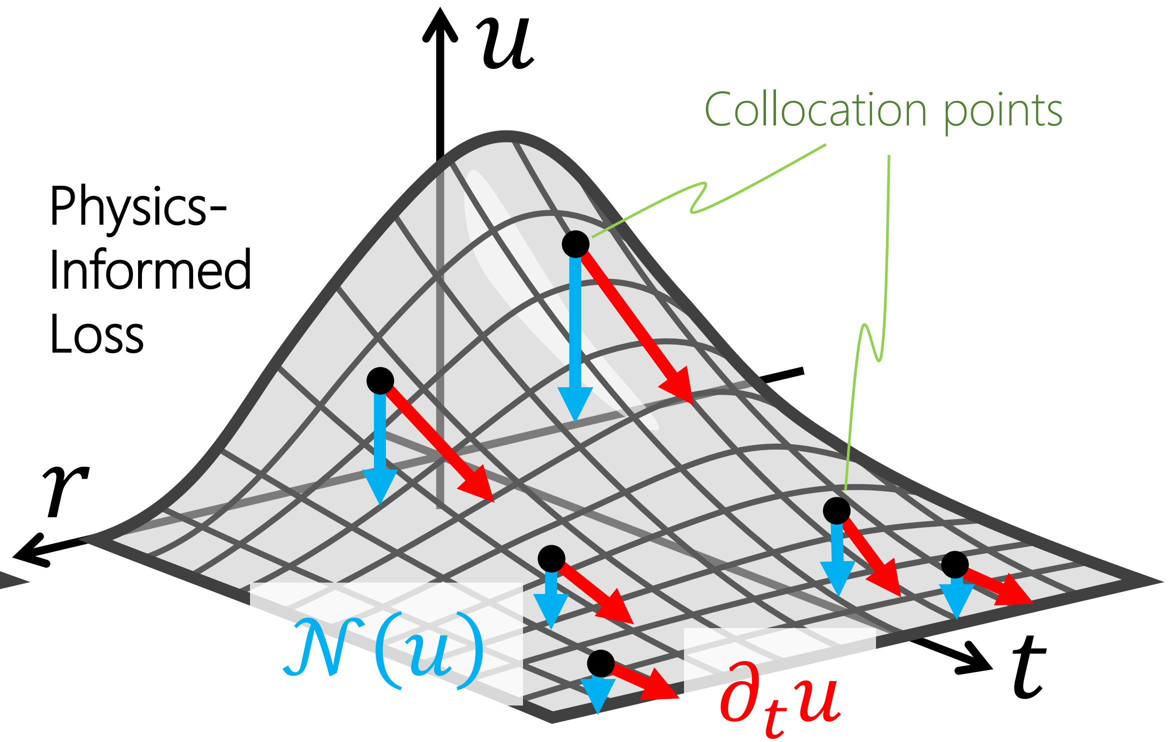

Recap of PINN and Neural Operator from a Differential Geometry Point of View

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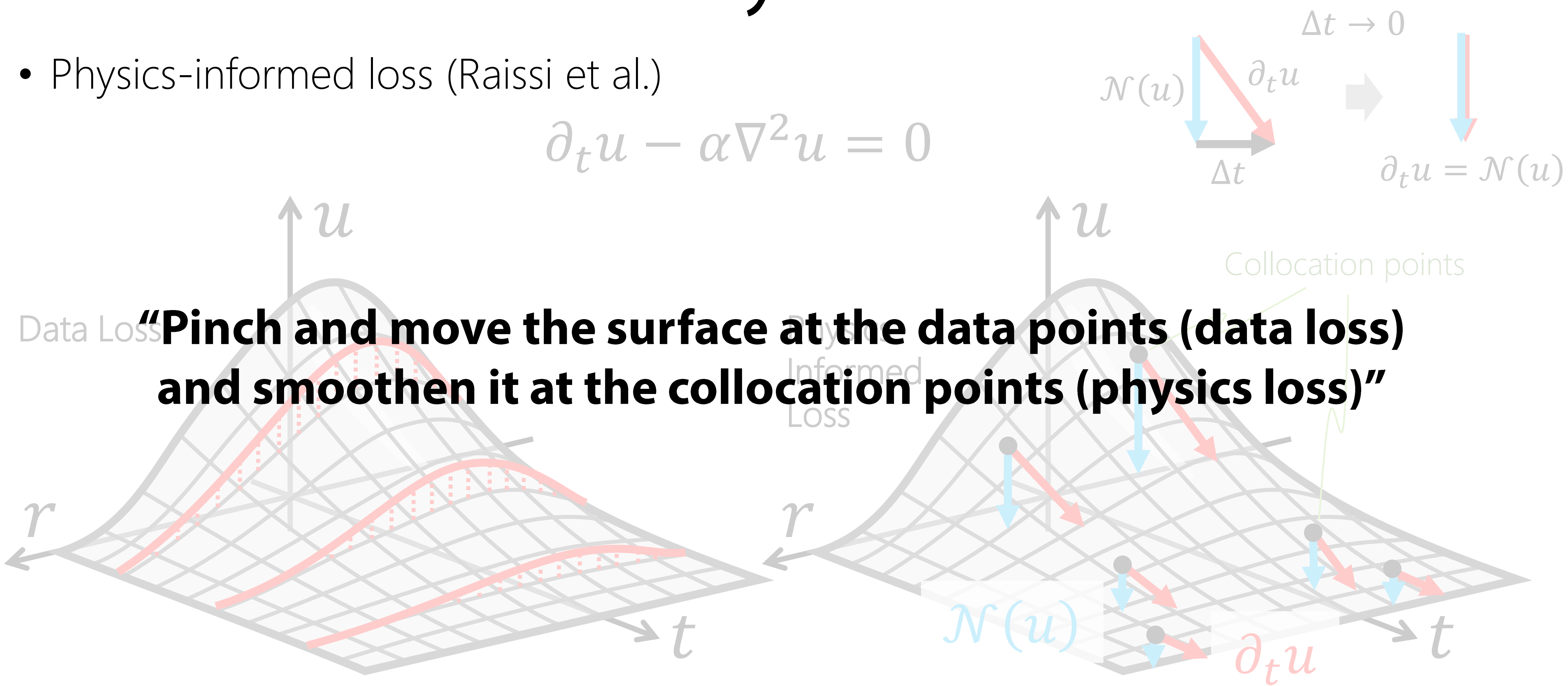
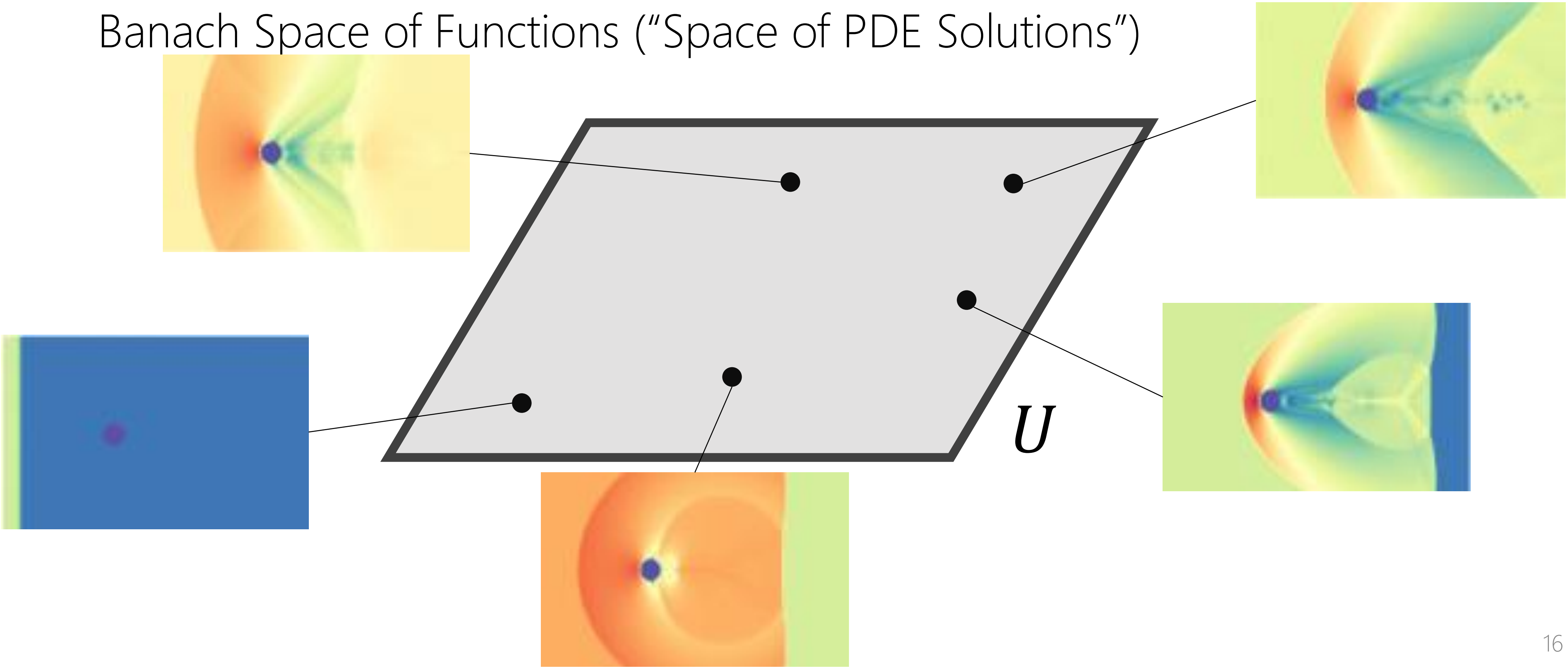


"Pinch and move the surface at the data points (data loss) and smoothen it at the collocation points (physics loss)"

Recap of PINN and Neural Operator from a Differential Geometry Point of View

- Neural Operators (Kovachki, Li, et al.)



Recap of PINN and Neural Operator from a Differential Geometry Point of View

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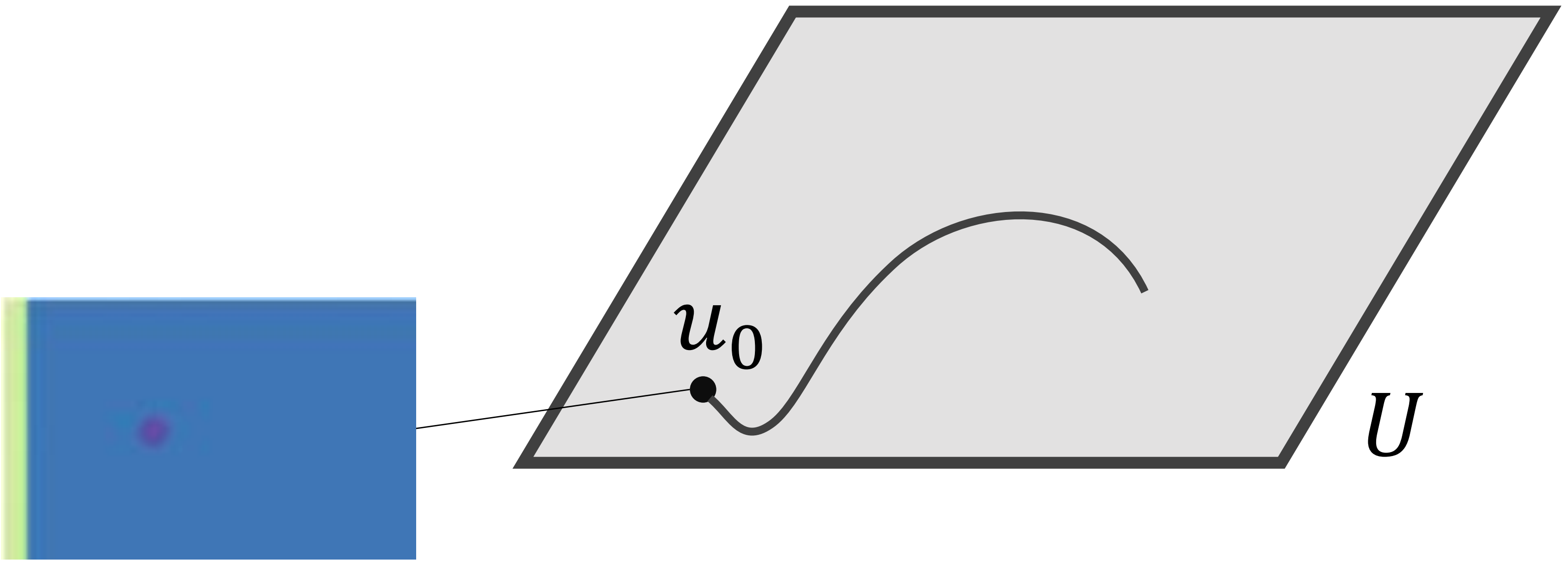
Banach Space of Functions ("Space of PDE Solutions")



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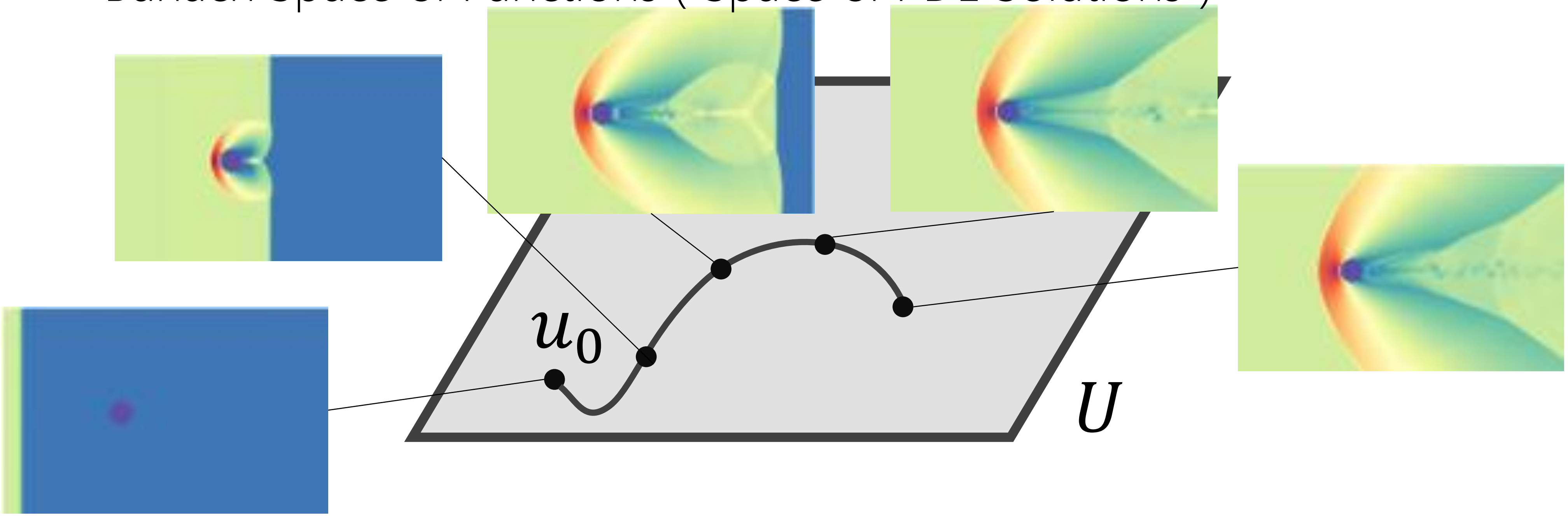

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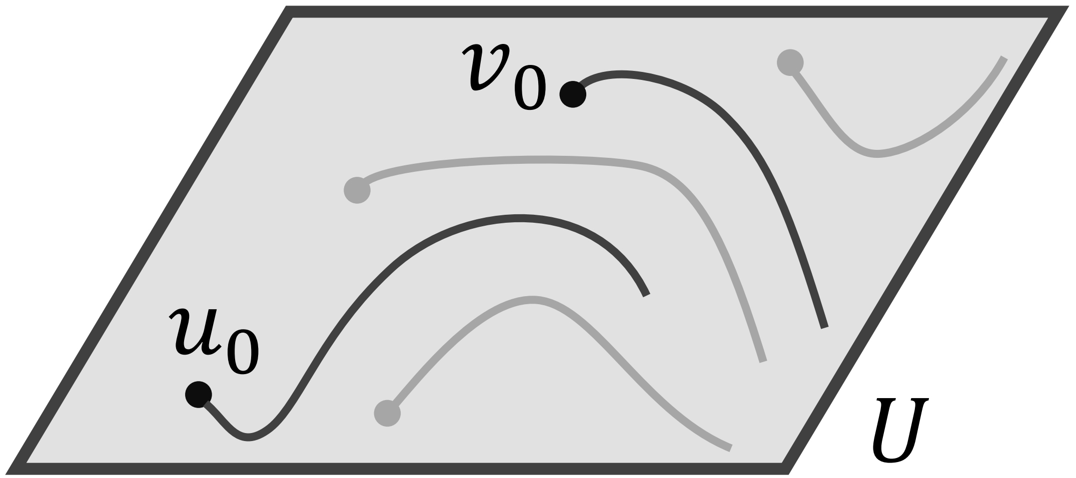

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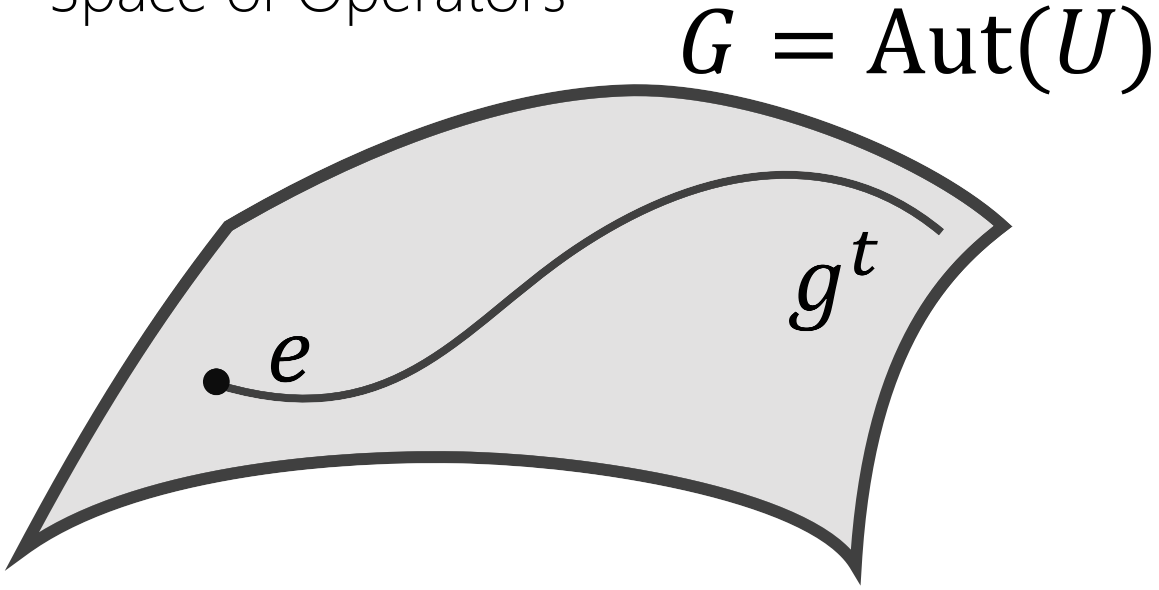
Space of Operators



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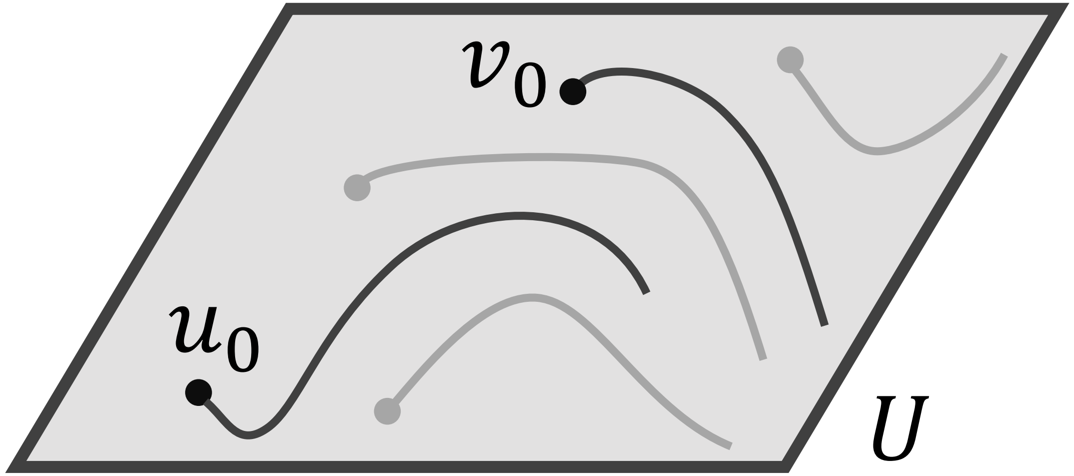

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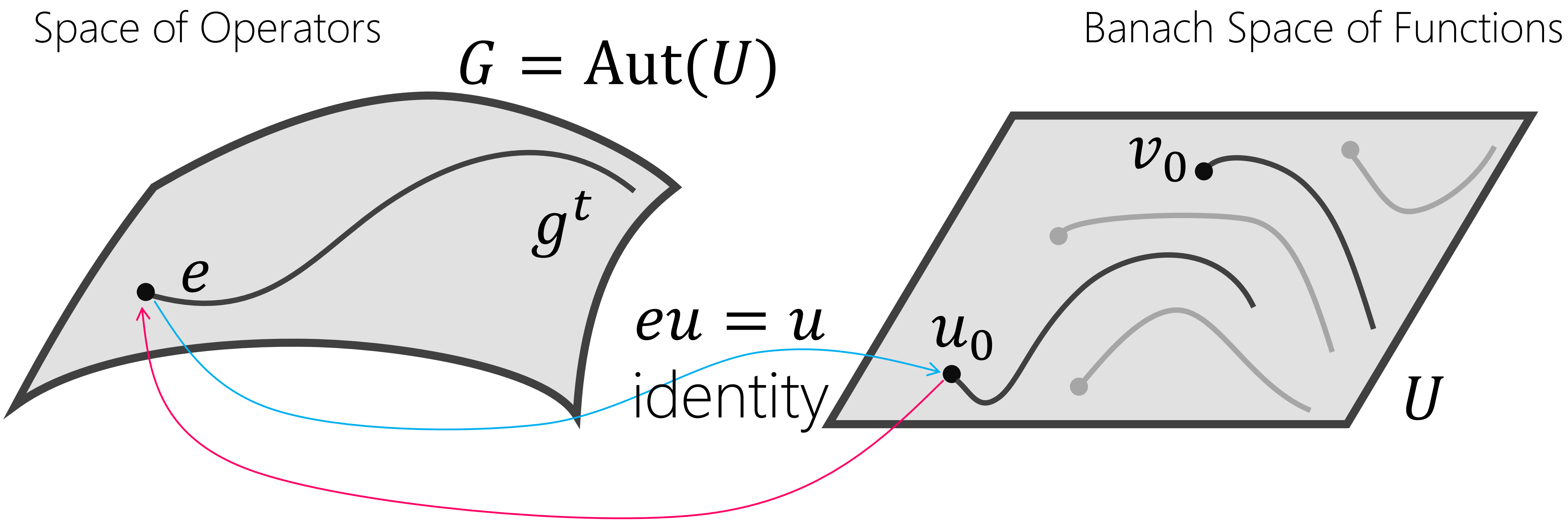

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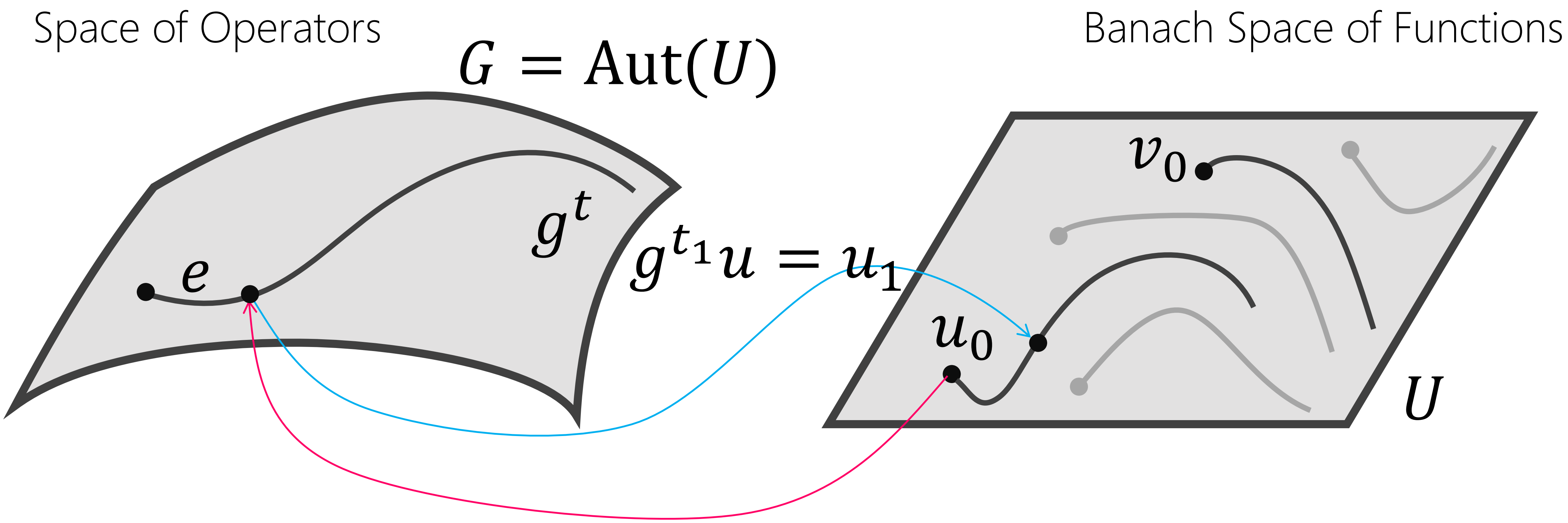

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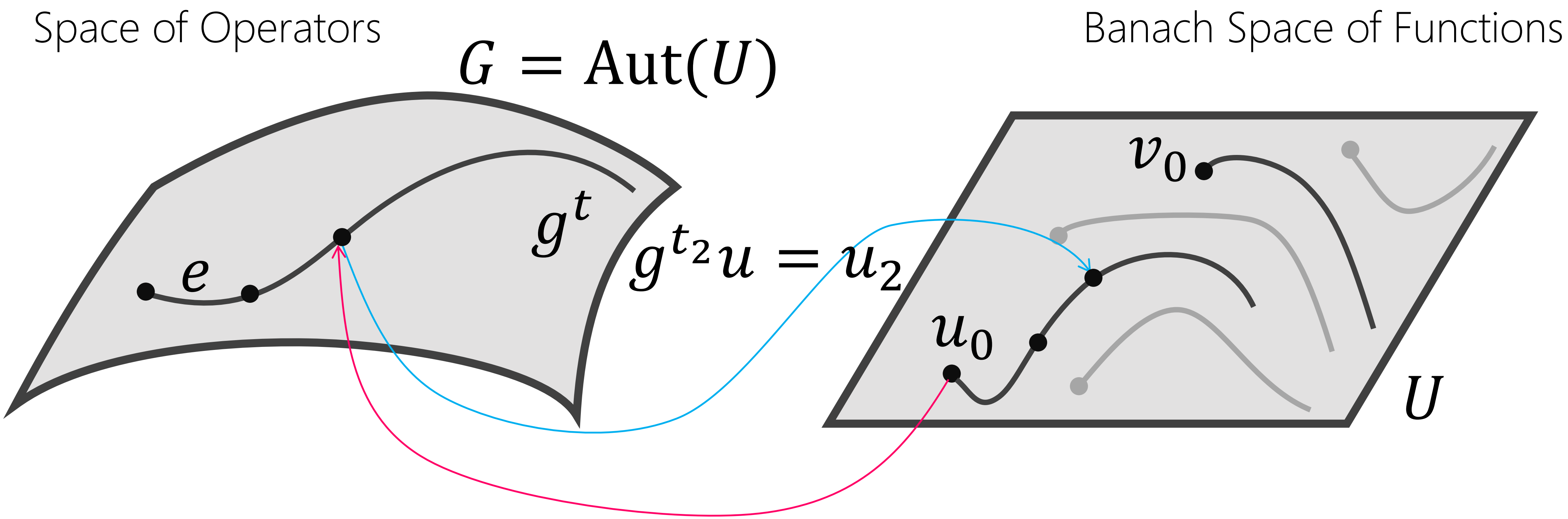

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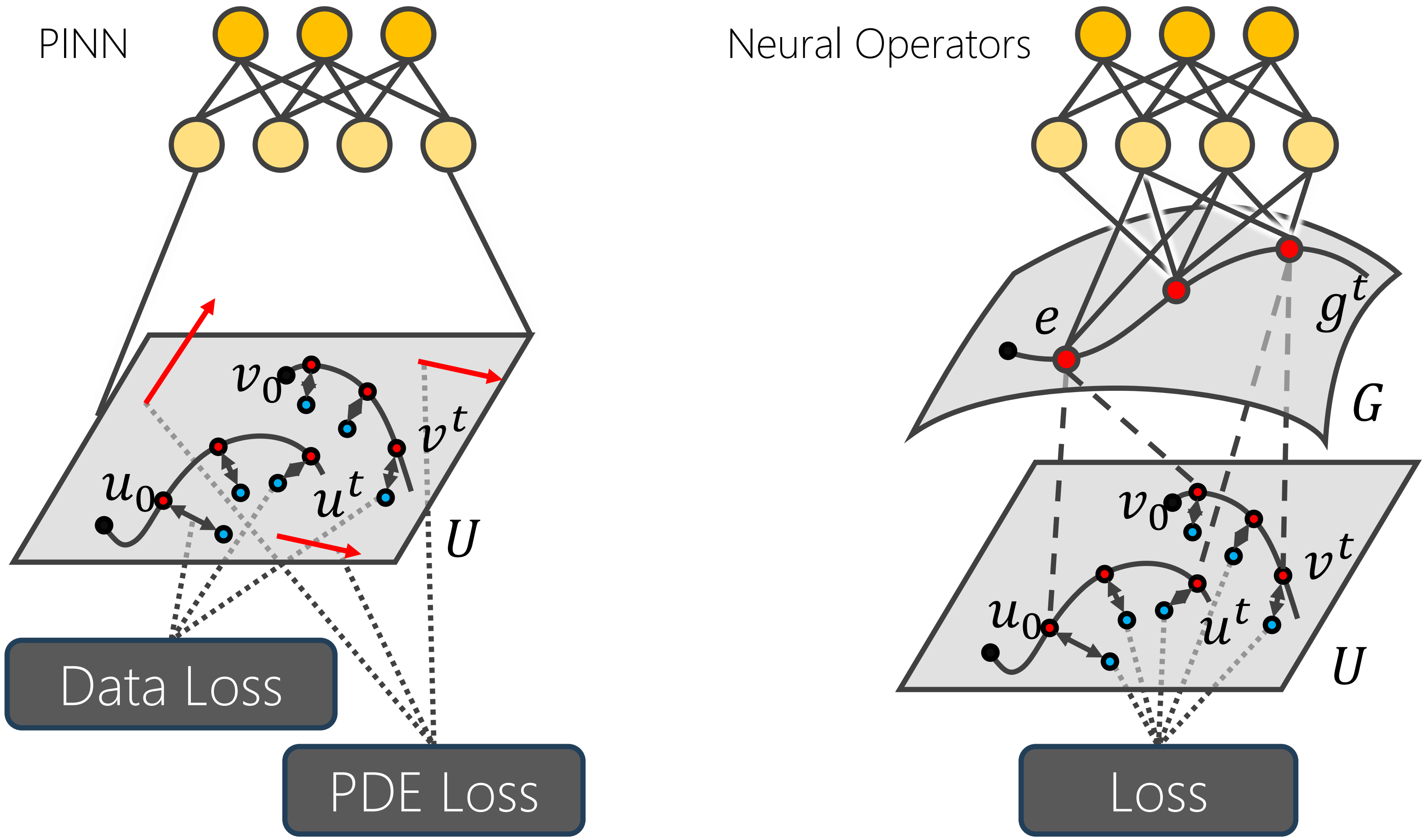


Re-thinking the Physics Learning

- PINN: Learning the solution function
    - Approximate the solution function using neural networks
    - Search space: Entire space of functions $\mathcal{U}$

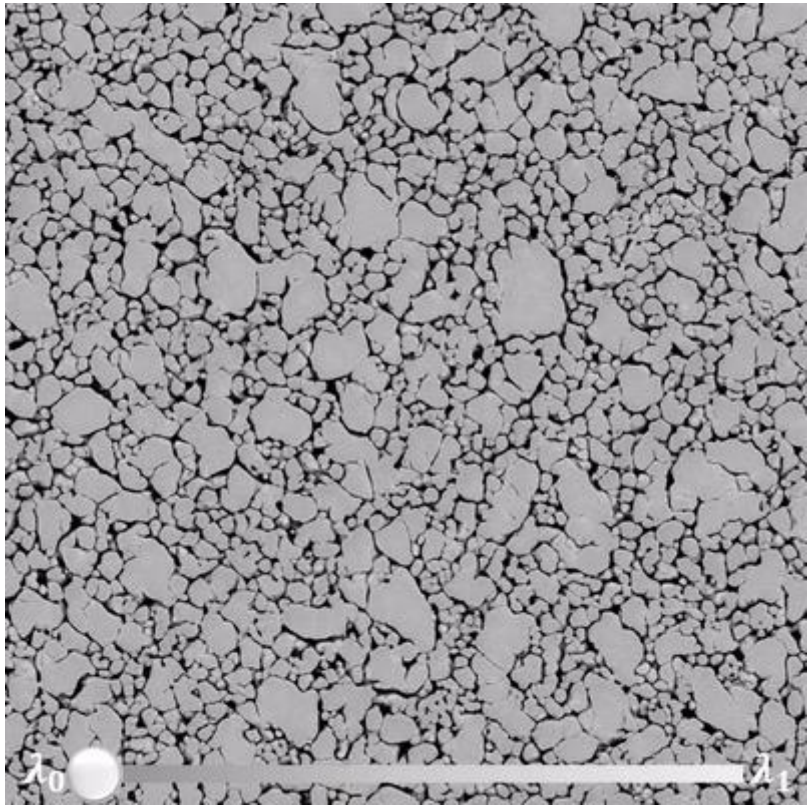
    - If IC/BC/other physical conditions change, the model needs to be retrained.
    - When the solution function u is nonlinear, the model is harder to fit with small data

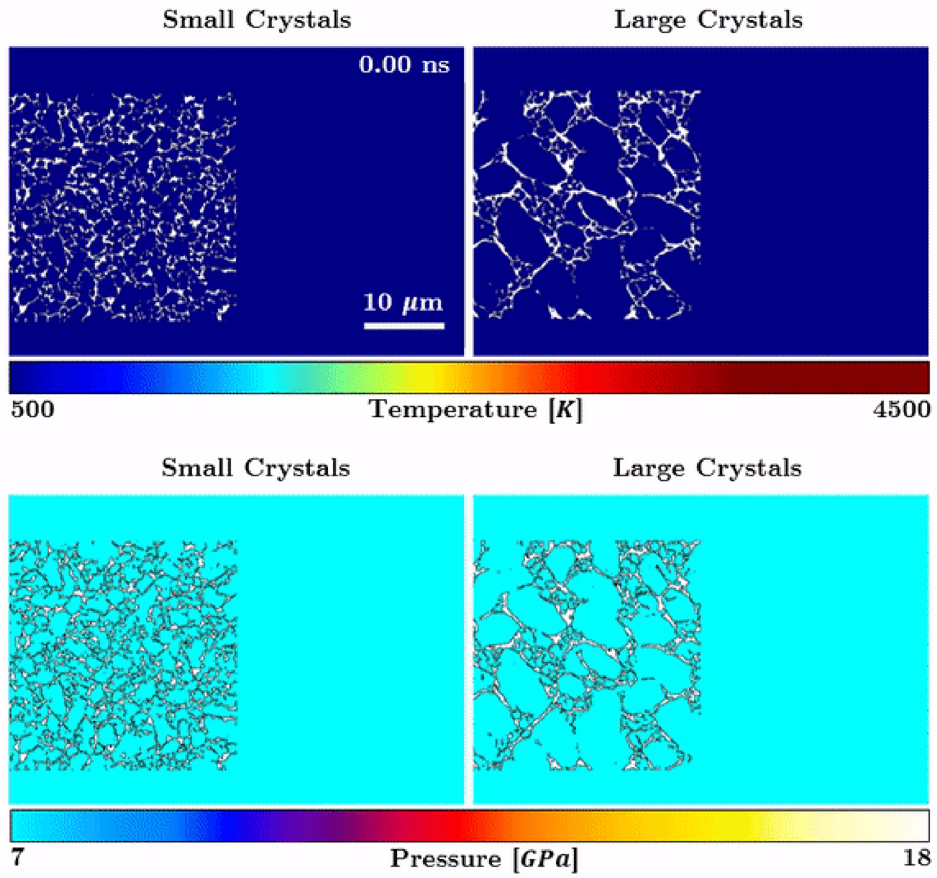
- Neural Operators: Learning the operator
    - Approximate the solution operator using neural networks
    - Search space: Space of operators $\mathcal{G}$

    - Model is still valid for different IC/BC/physical parameters
    - Relatively easier to learn nonlinear dynamics

Physics-Aware Recurrent CNNs (PARC)

- Initial & boundary value problems





Chun et al. (2020) https://www.nature.com/articles/s41598-020-70149-0

Morphology

$$\frac{\partial X}{\partial t} = f(X, \mu) + \epsilon$$

Quantities of interest

(e.g., temperature & pressure)

Deep neural network

model parameters

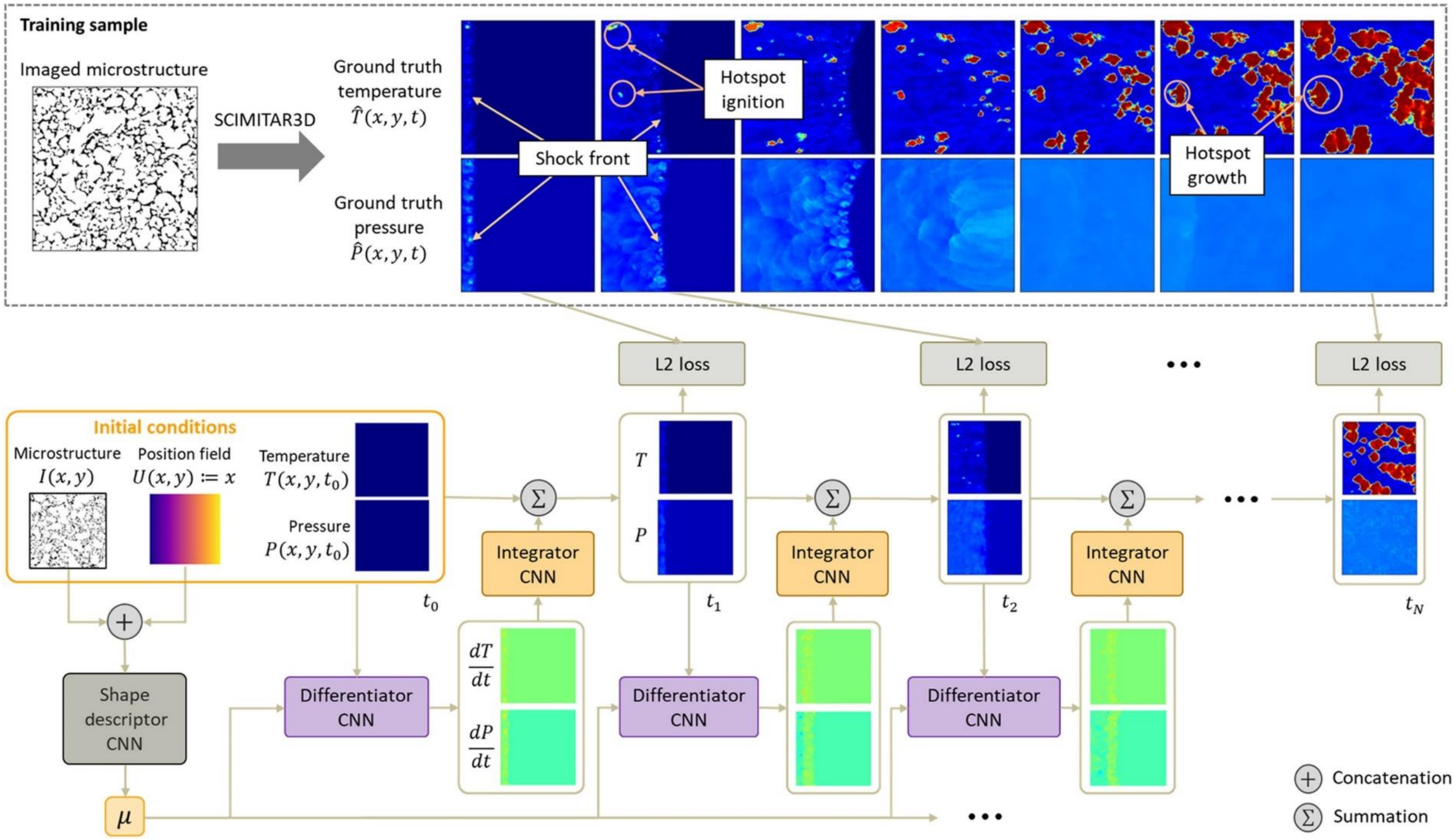
$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

stochastic noise + prediction error

$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

$$X(t + \Delta t) = X(t) + \int_0^{\Delta t} f(X, \mu \mid \theta) dt$$

Physics-Aware Recurrent CNNs (PARC)



$$\frac{\partial X}{\partial t} = f(X, \mu \mid \theta) + \varepsilon$$

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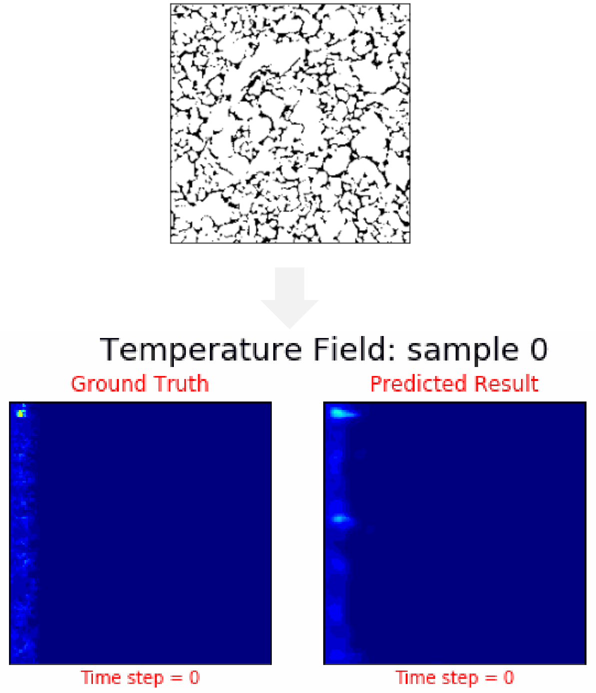
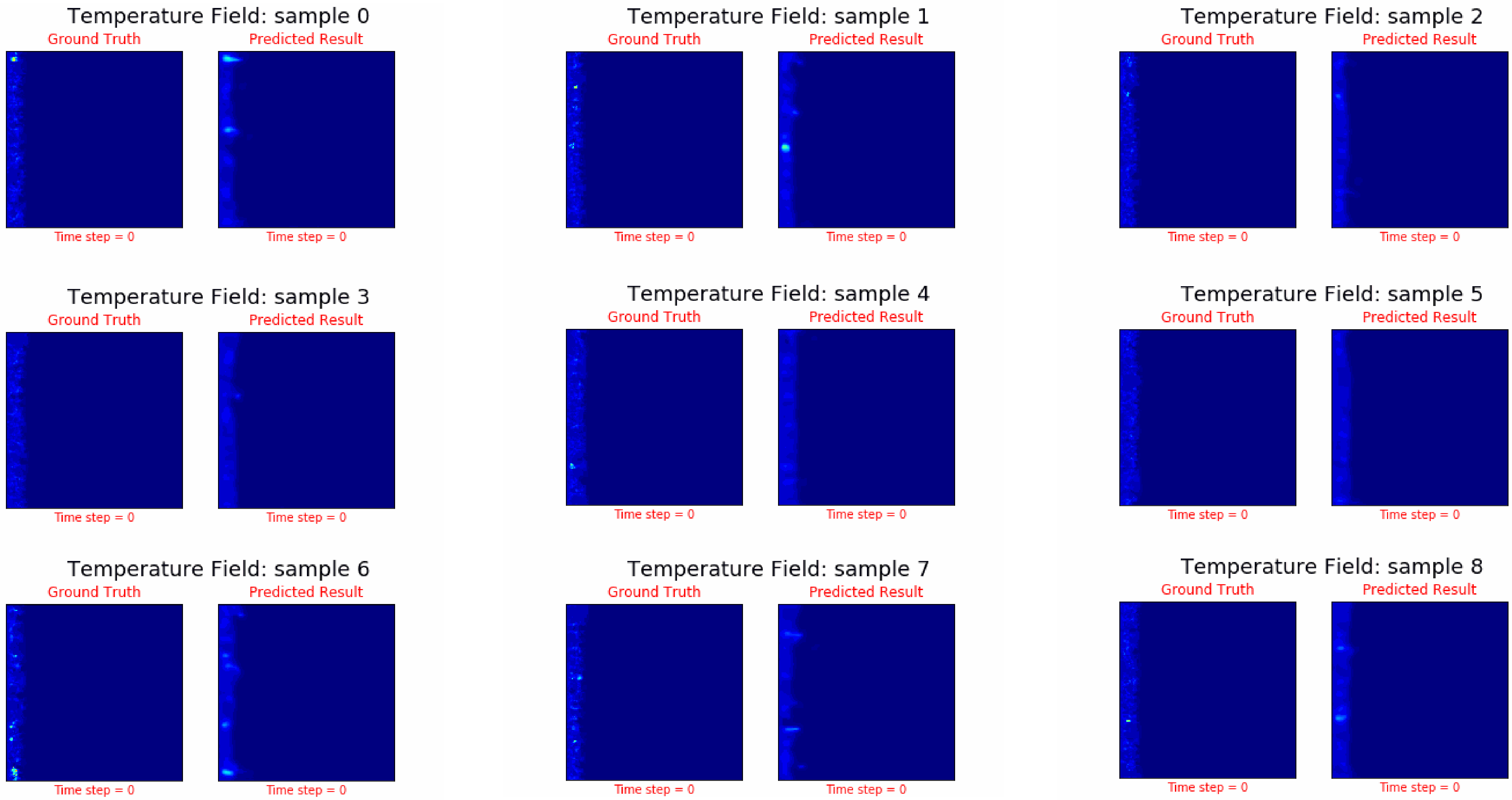


Nguyen et al. (2023a). https://www.science.org/doi/10.1126/sciadv.add6868



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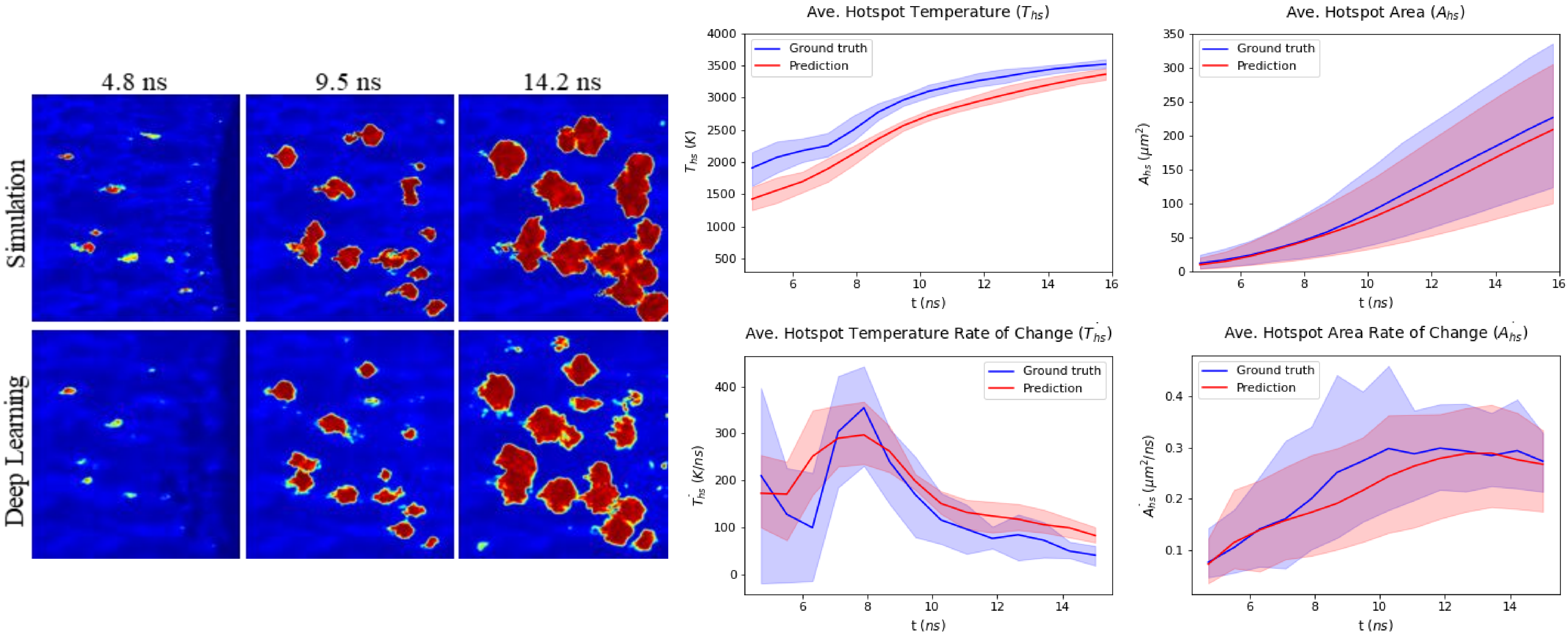
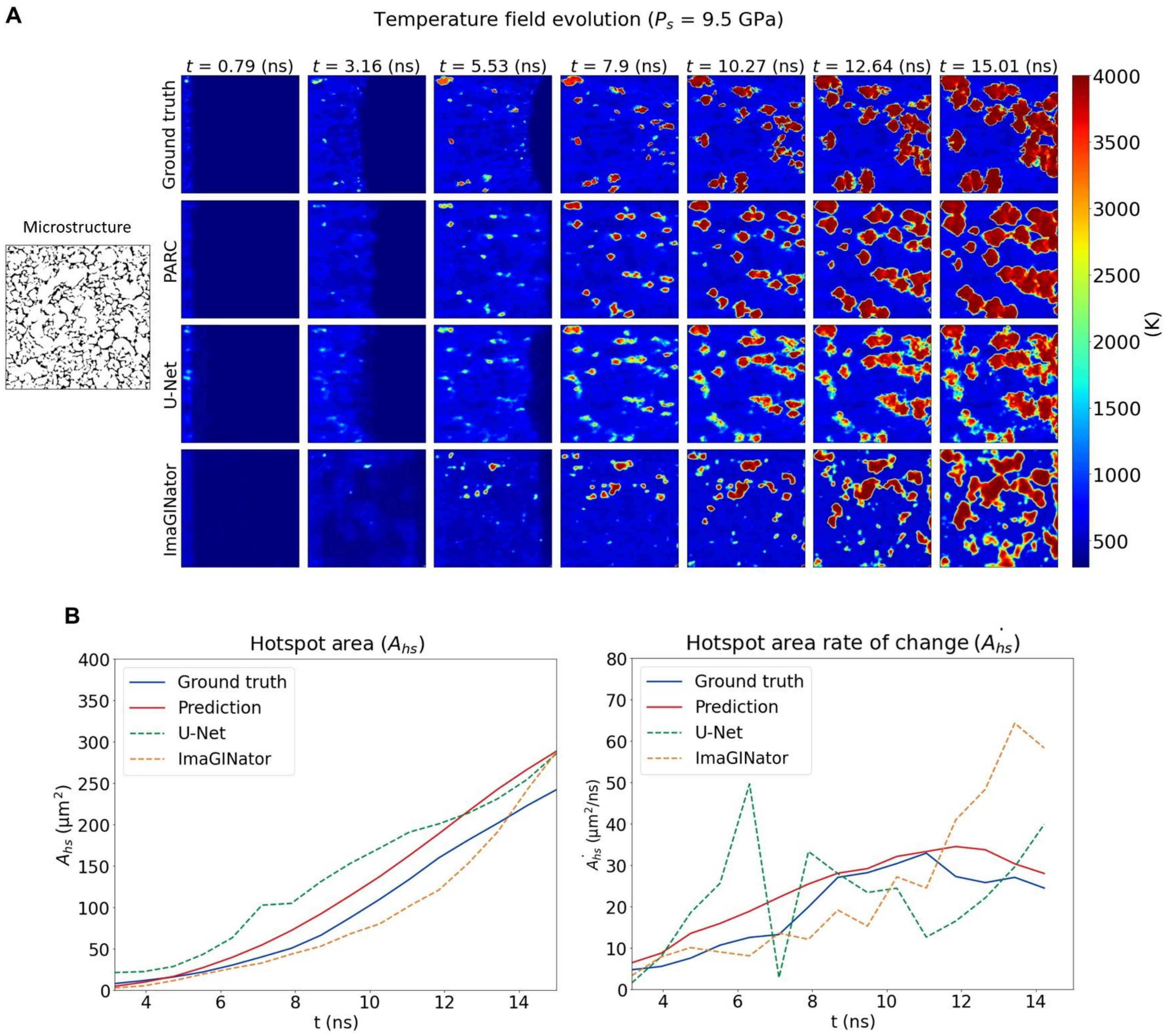


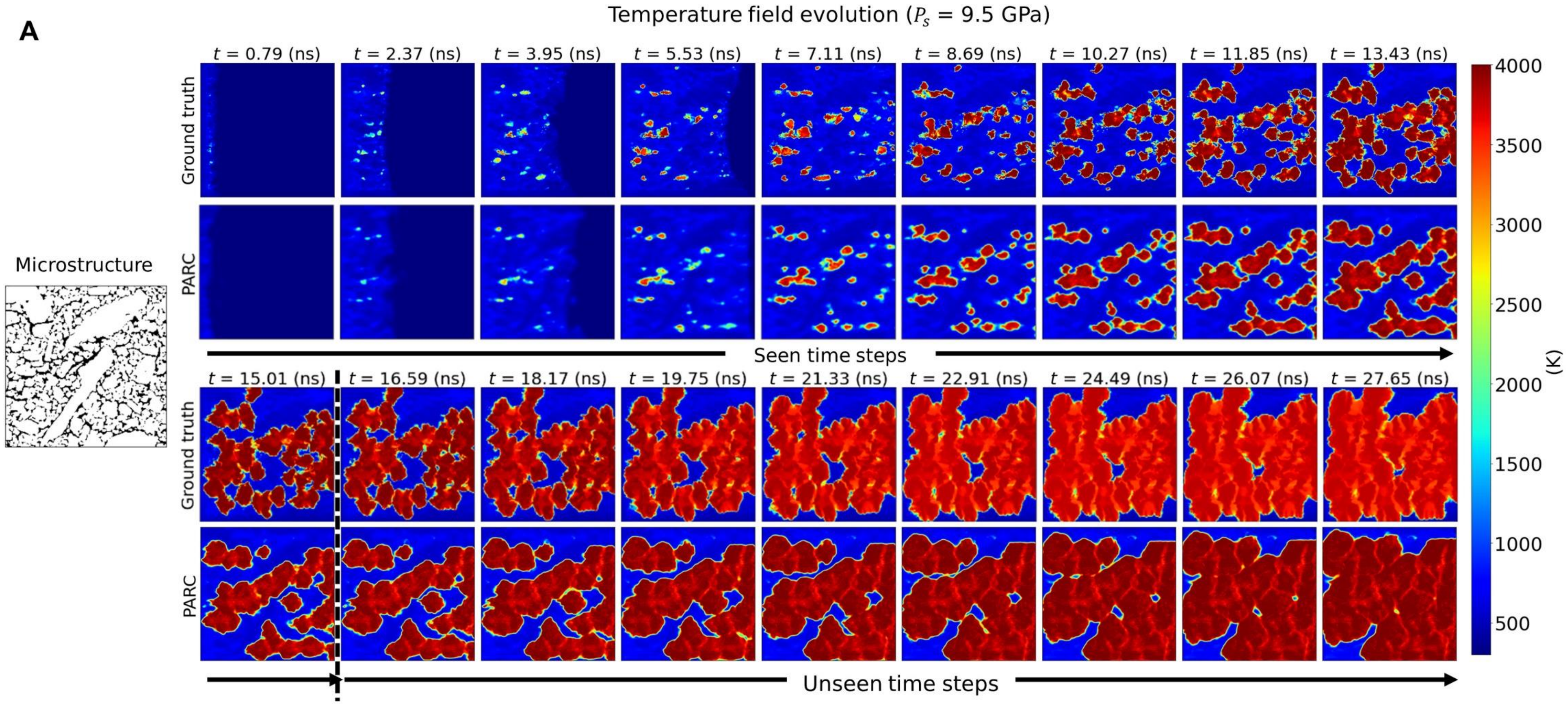
https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Aware vs Physics-Naïve



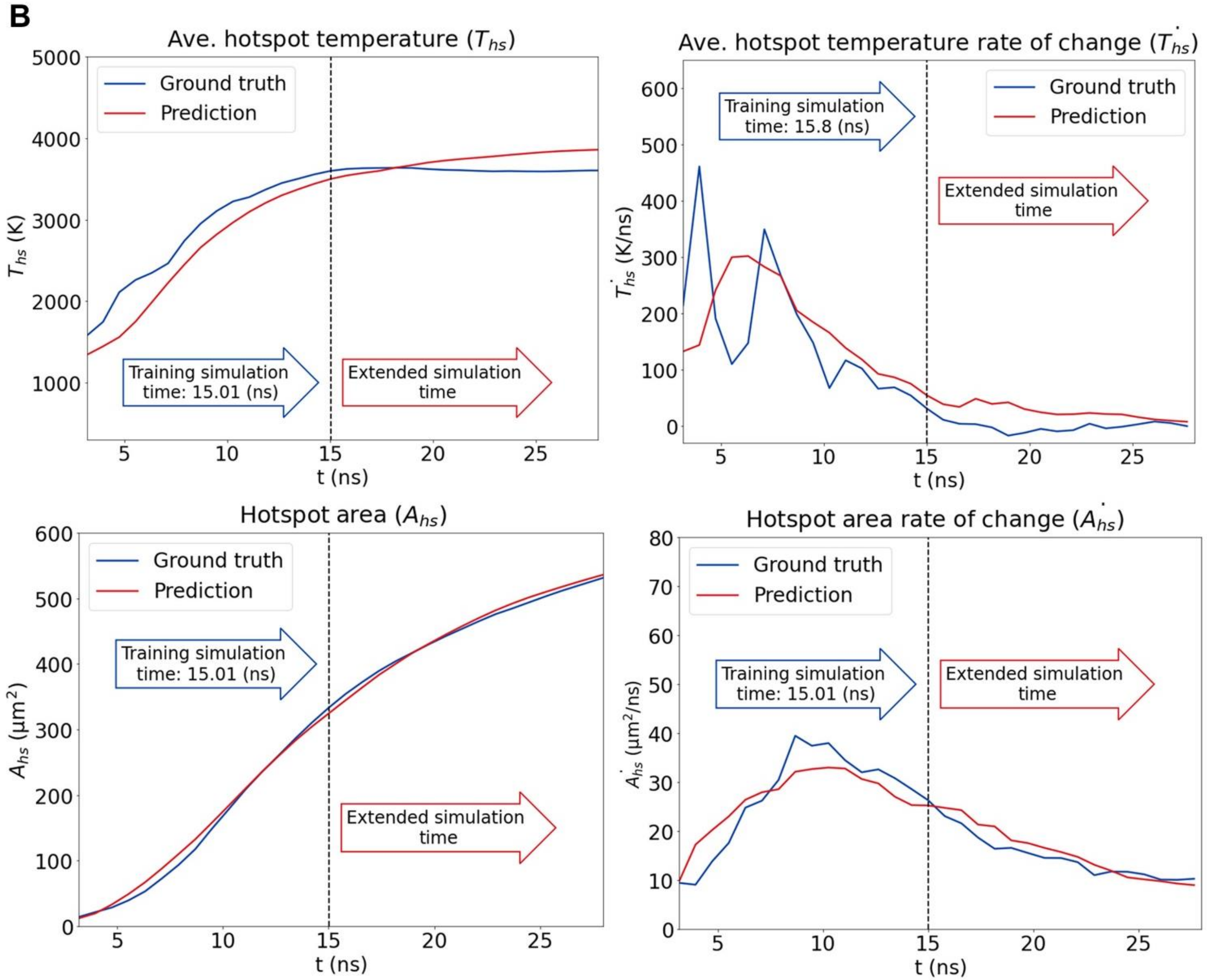
https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Awareness



https://www.science.org/doi/10.1126/sciadv.add6868

Physics-Awareness



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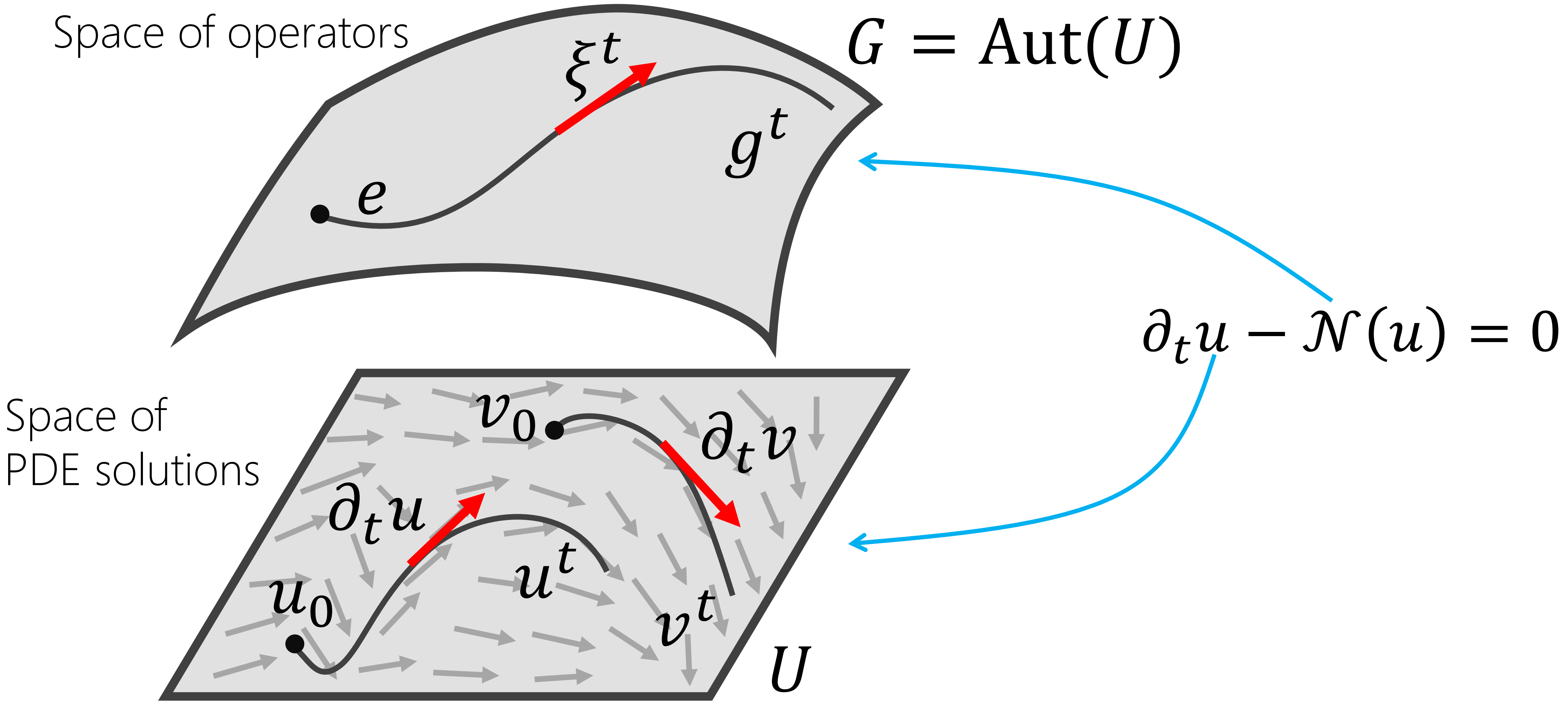
Differential Geometry Perspective



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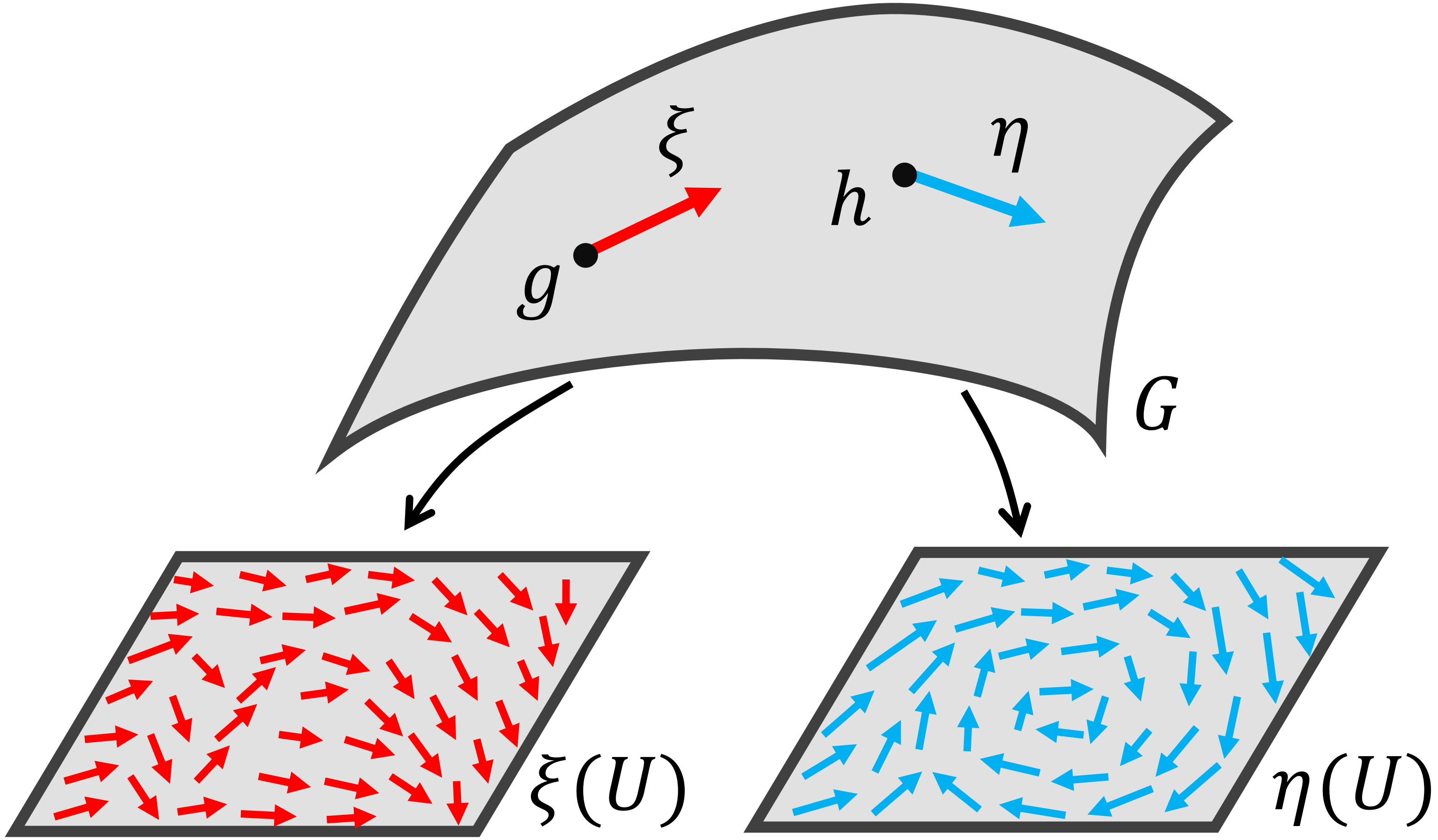
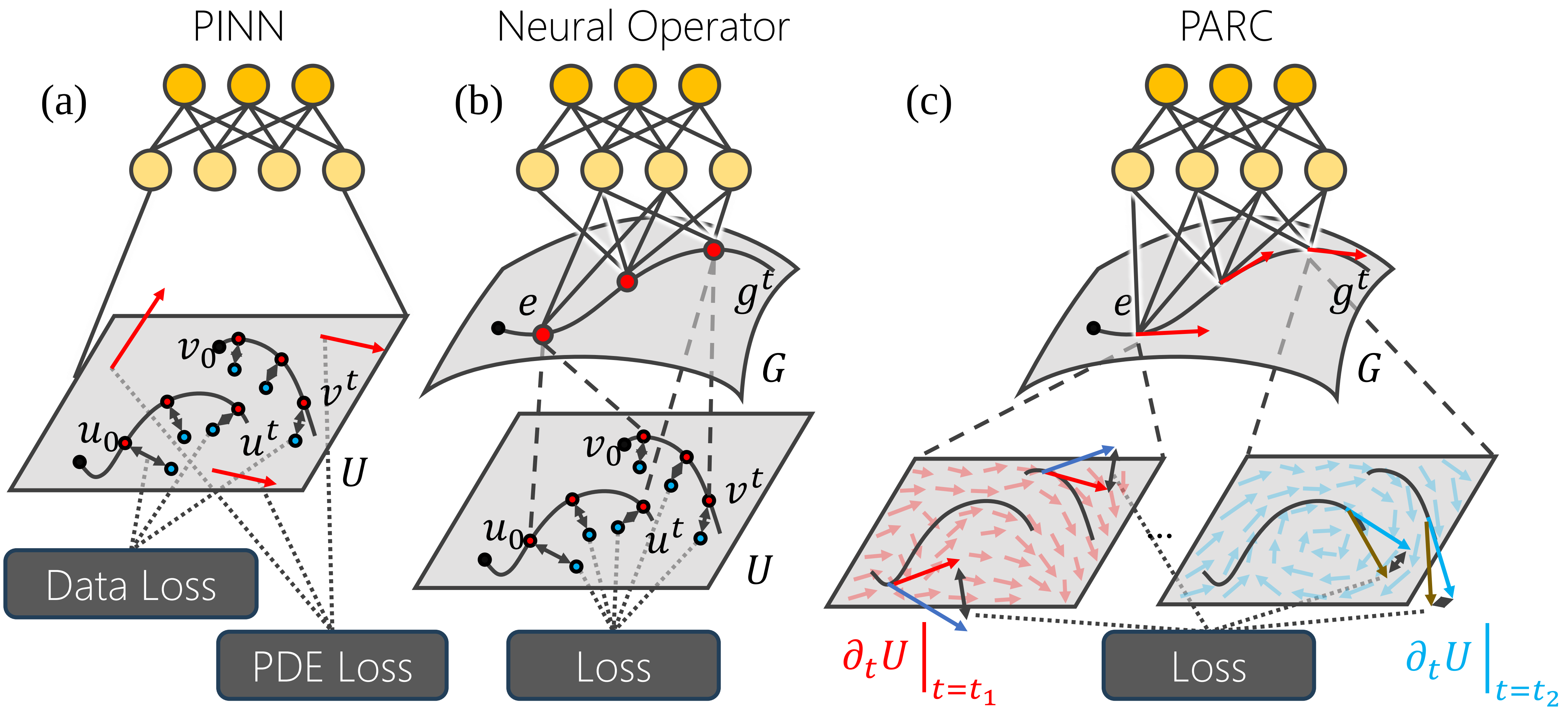
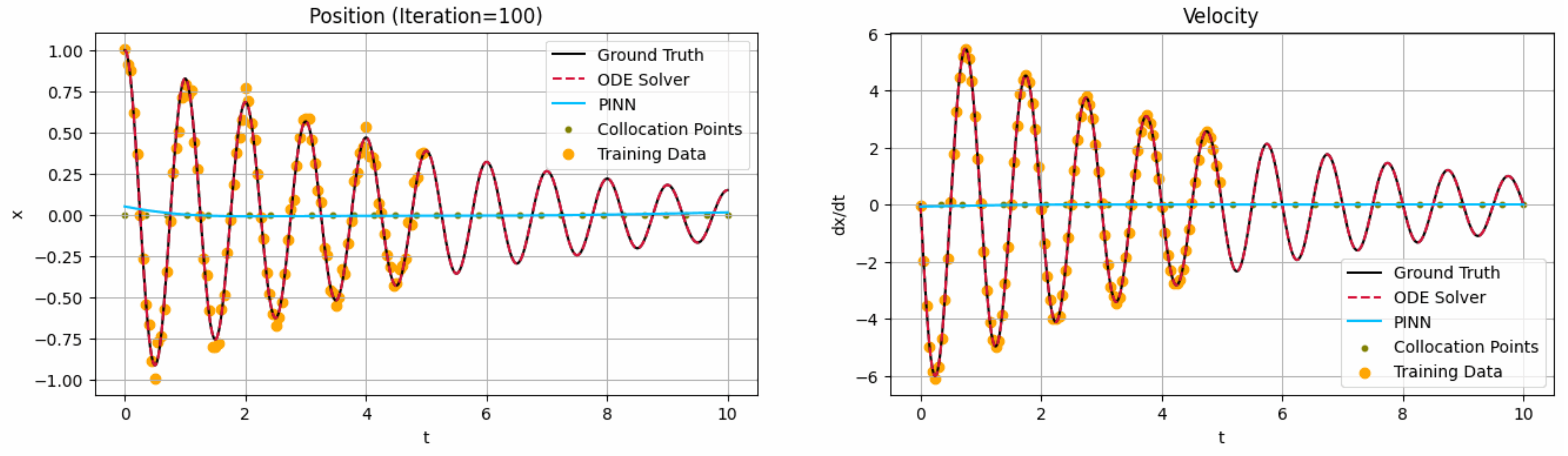


Different Ways to Inform Physics

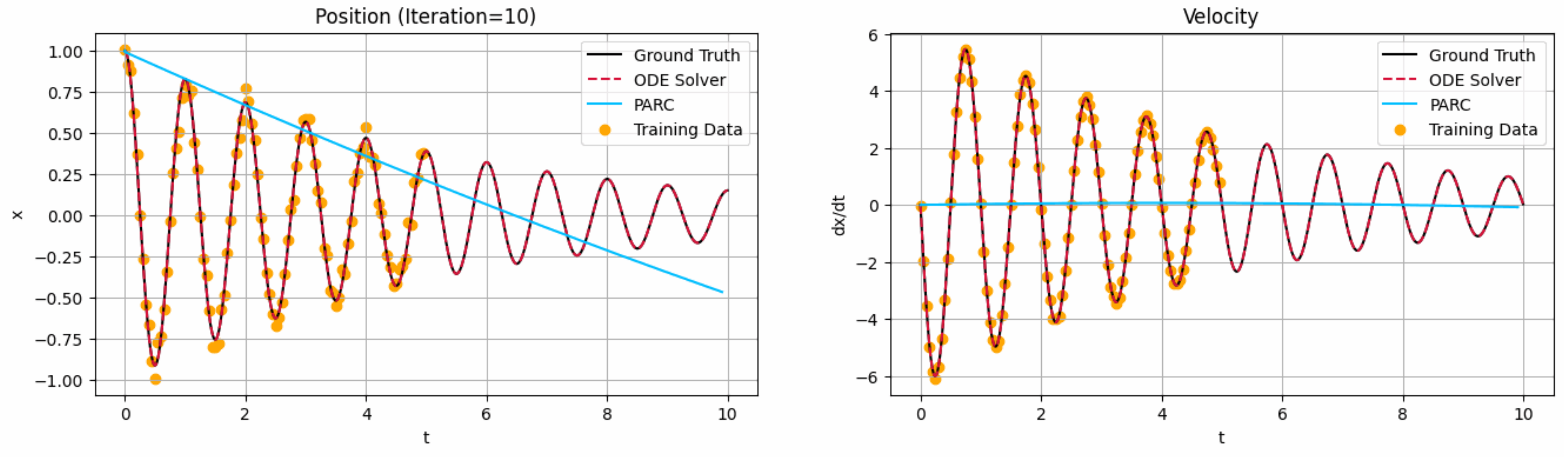


Learning on the Hilbert Space Vs. Learning on the Operator Manifold

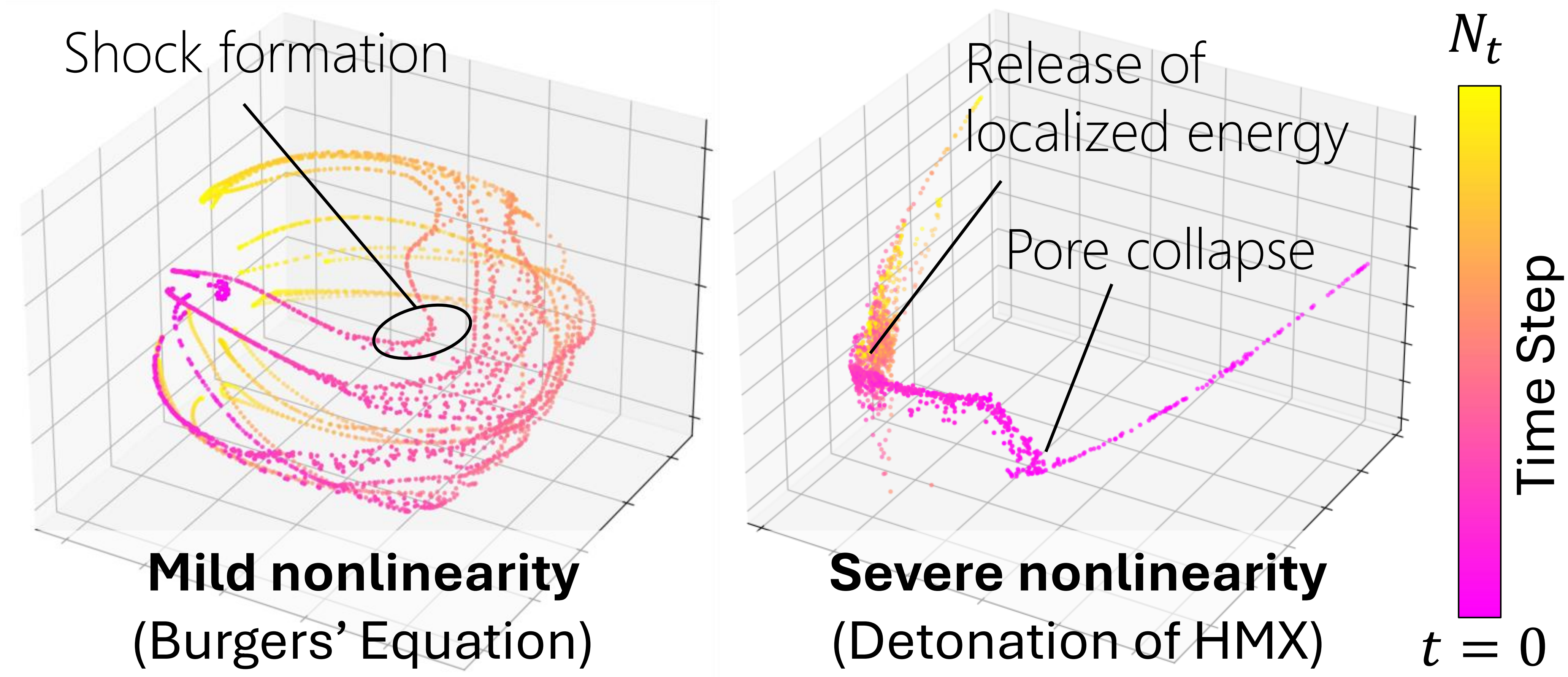
Physics-Informed Neural Network
(3 hidden layers – 256, 256, 256)



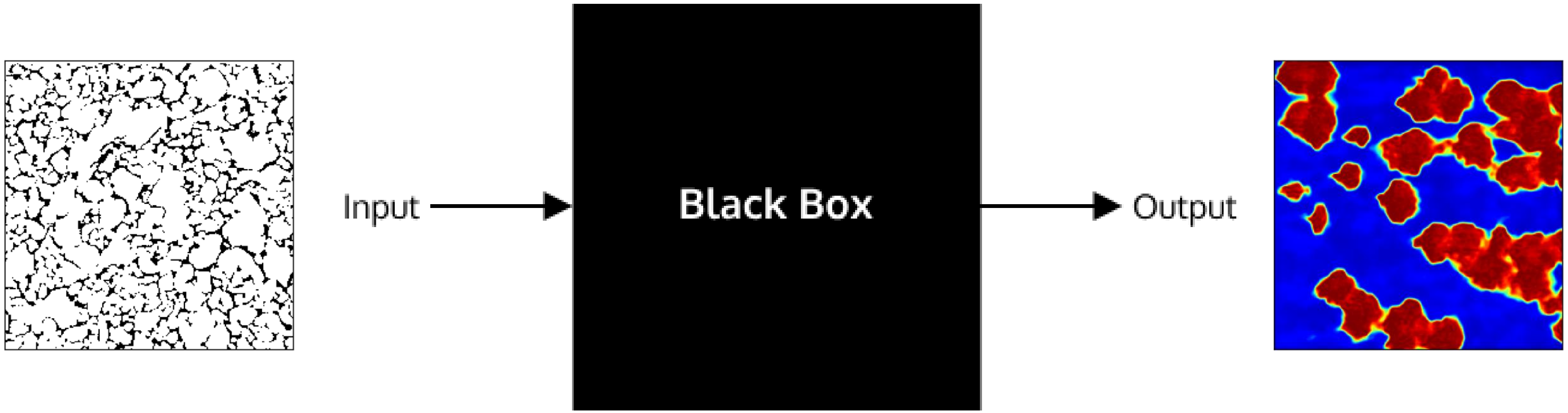
Physics-Aware Recurrent Conv.
(2 hidden layers – 16, 32)



Geometry of Extreme Dynamics



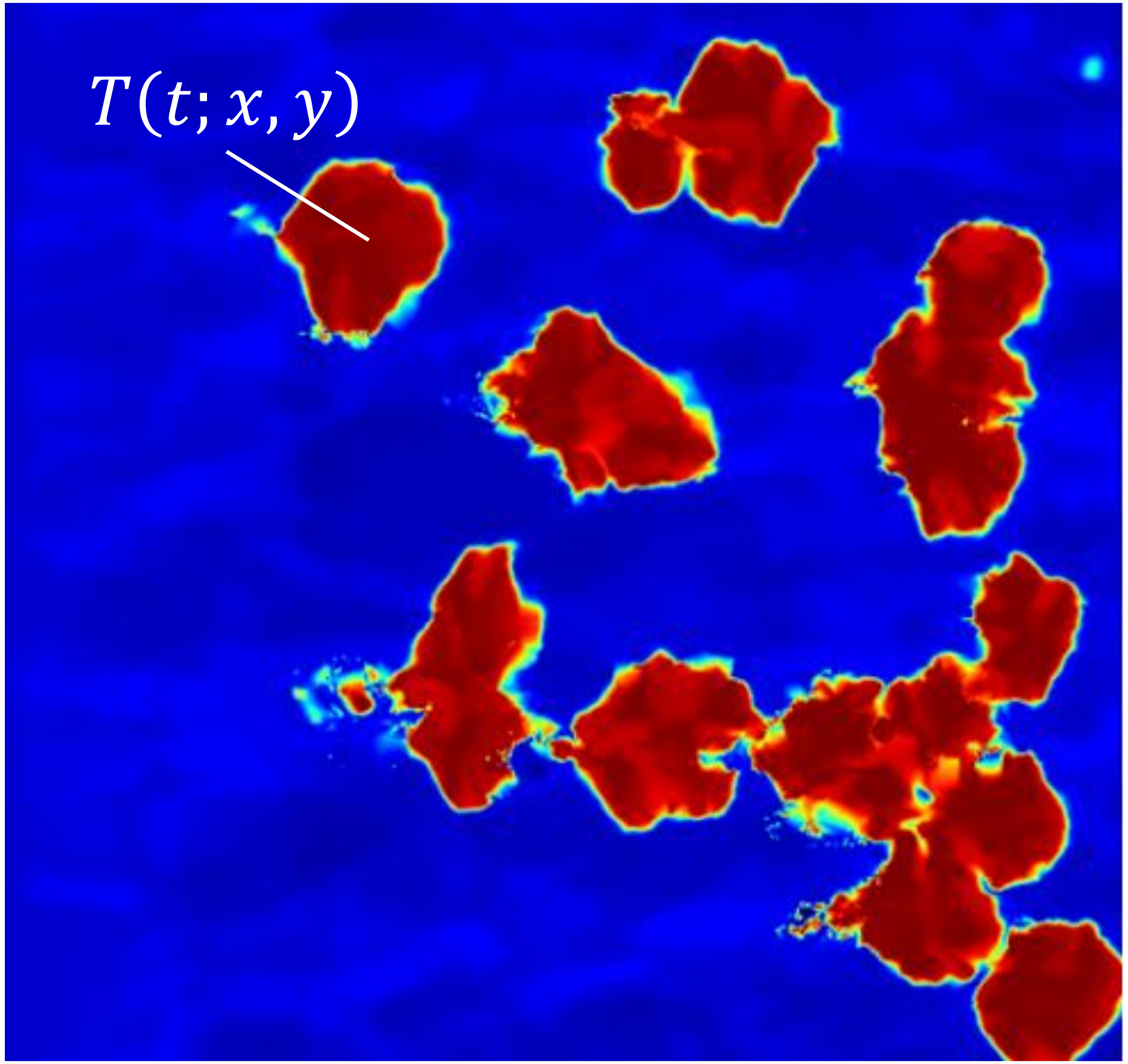
What does PARC see in microstructure images?

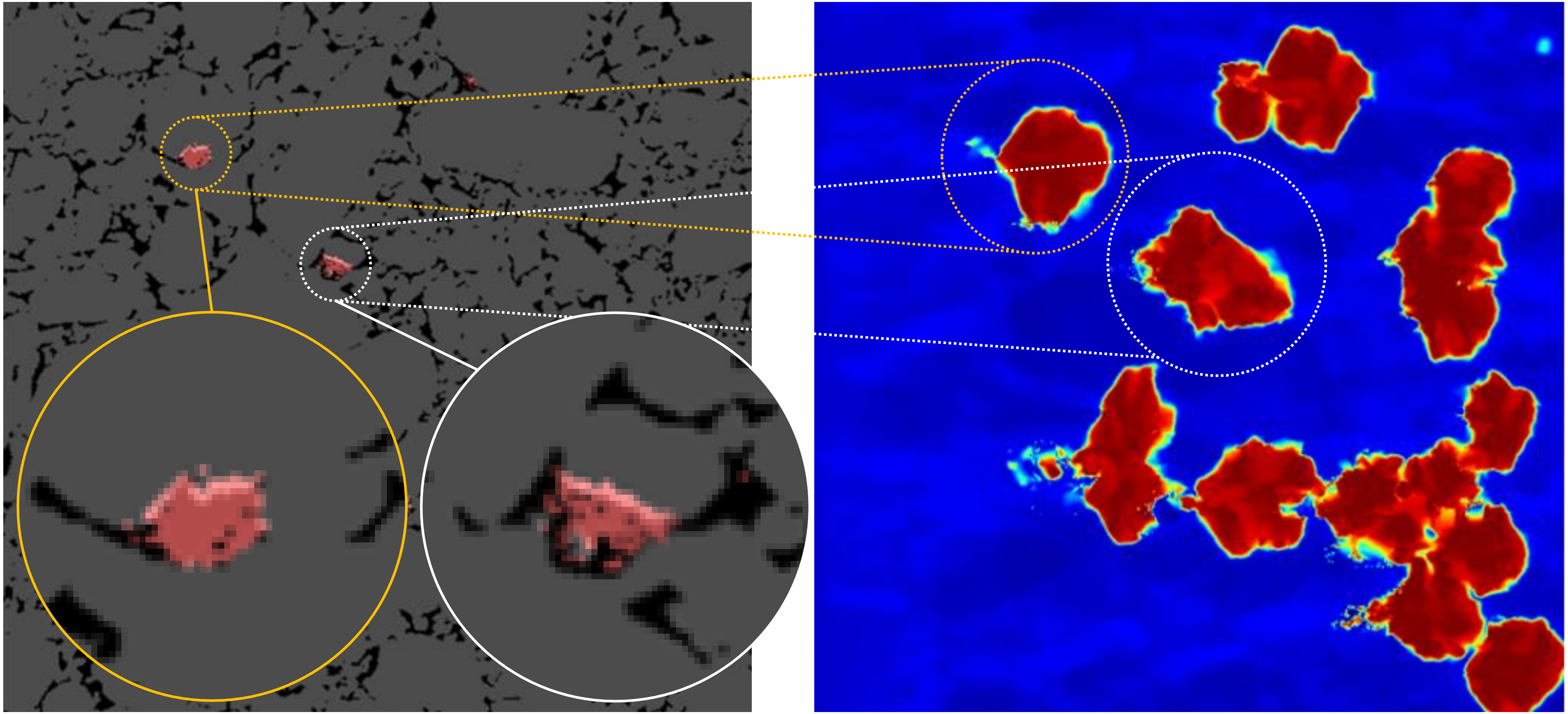


Saliency Map

Which element in the microstructure had the biggest influence on the hotspot formation?

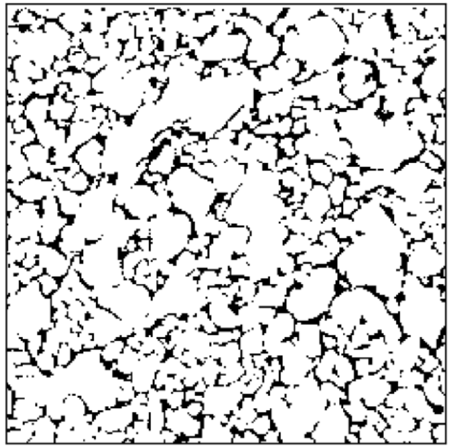
$$\frac{\partial T}{\partial \mu(x,y)}$$



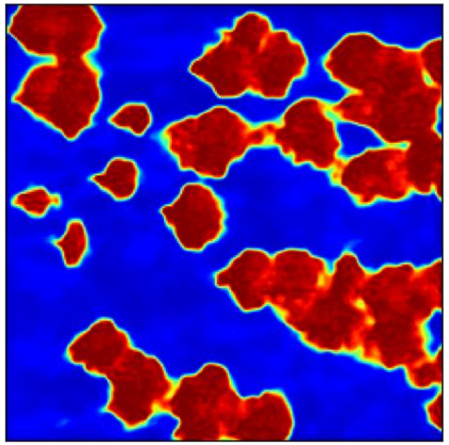


Saliency Map

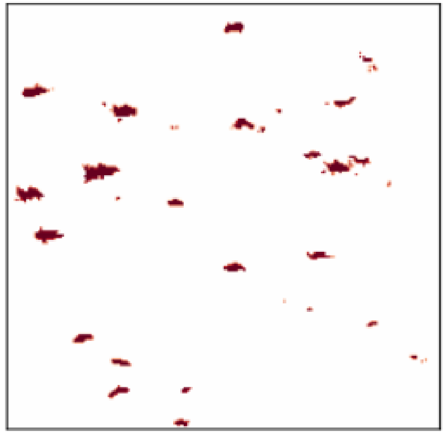
Microstructure $\mu(x, y)$



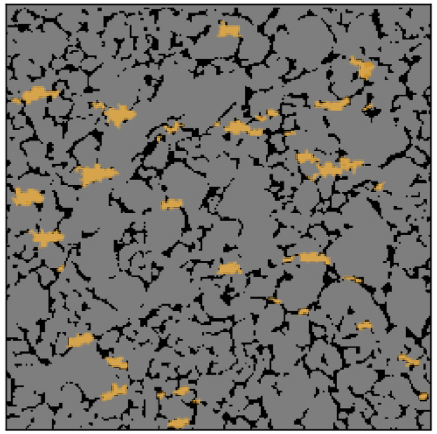
Temperature field $\boldsymbol{T}(\boldsymbol{x}, \boldsymbol{y})$

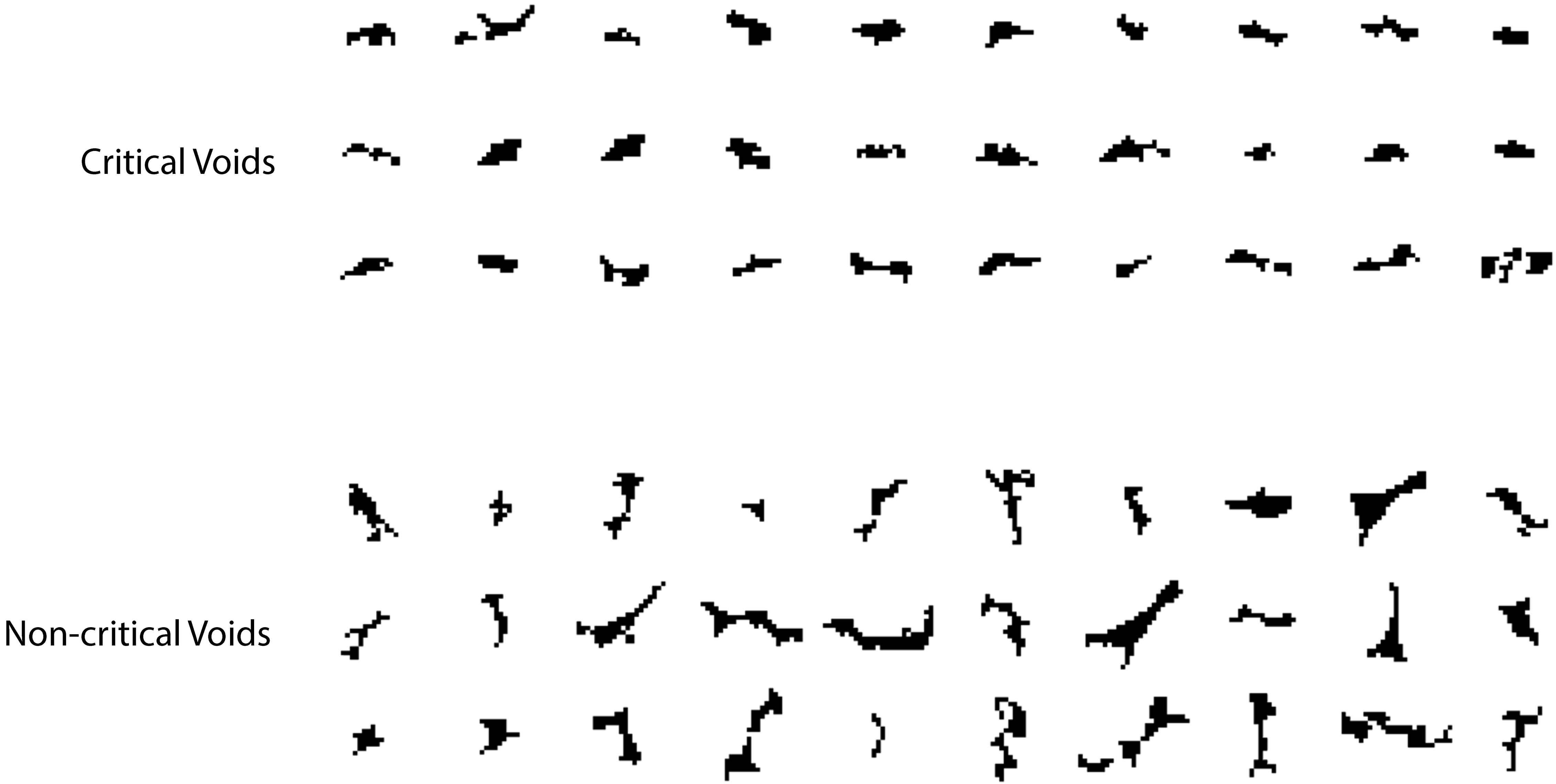


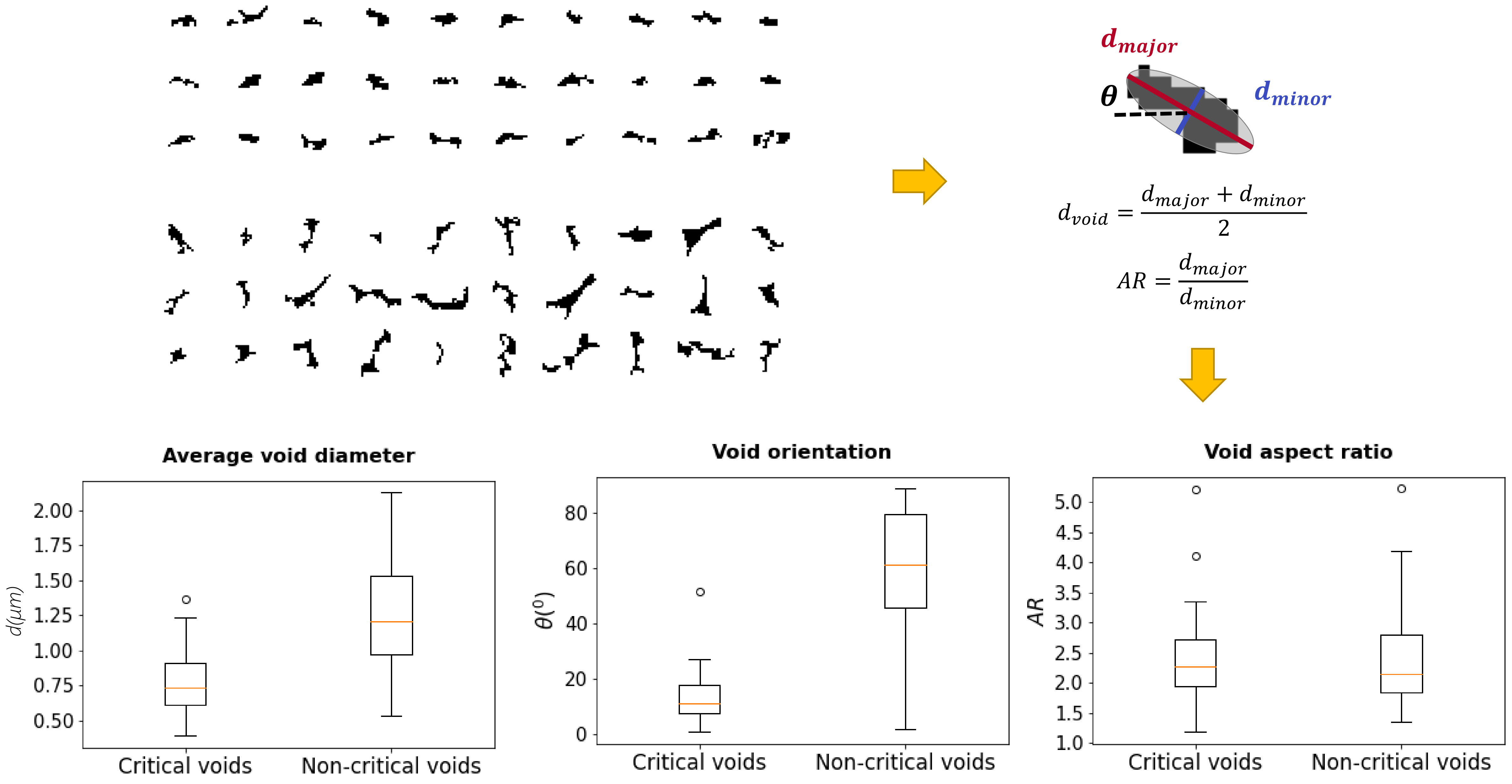
Saliency map $G(x, y)$



Saliency map superimposed on microstructure



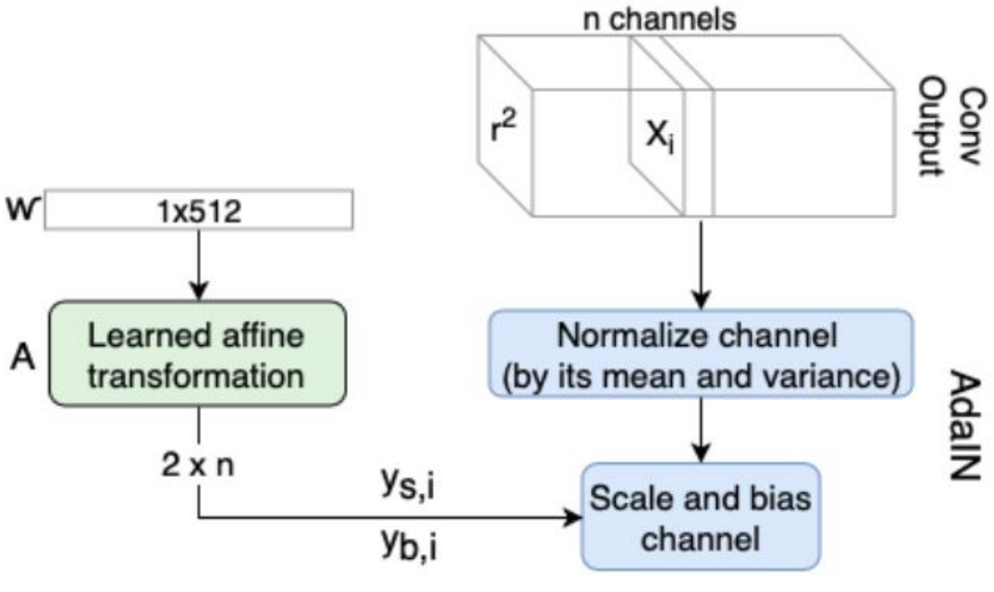

Critical Voids
Non-critical Voids



d_major
θ
d_minor
d_void = (d_major + d_minor) / 2
AR = d_major / d_minor
Average void diameter
d(μm)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
Critical voids
Non-critical voids
Void orientation
θ(°)
80
60
40
20
0
Critical voids
Non-critical voids
Void aspect ratio
AR
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Critical voids
Non-critical voids

PARCel – Extending PARC to other operating conditions

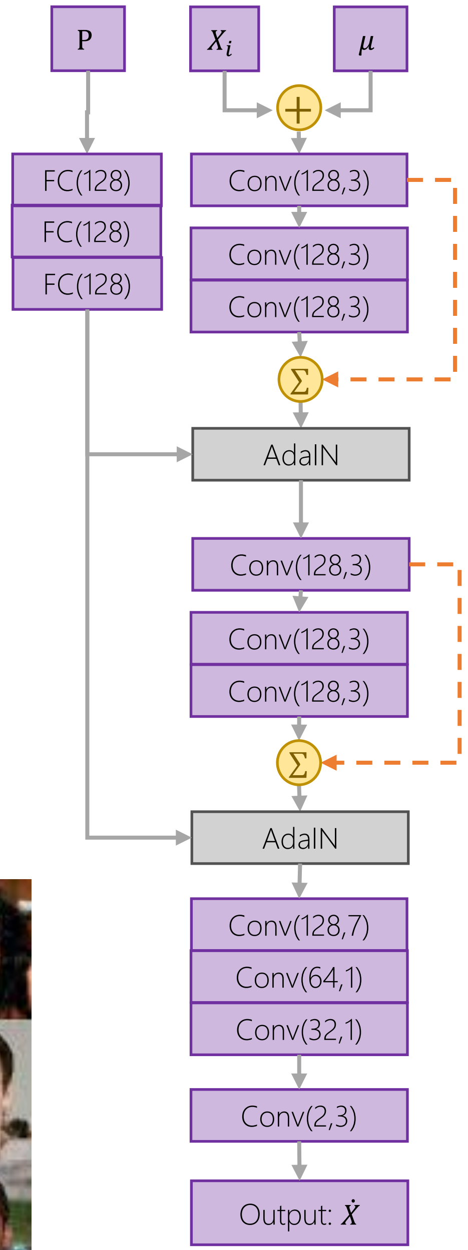
- "Style-vector" in StyleGAN



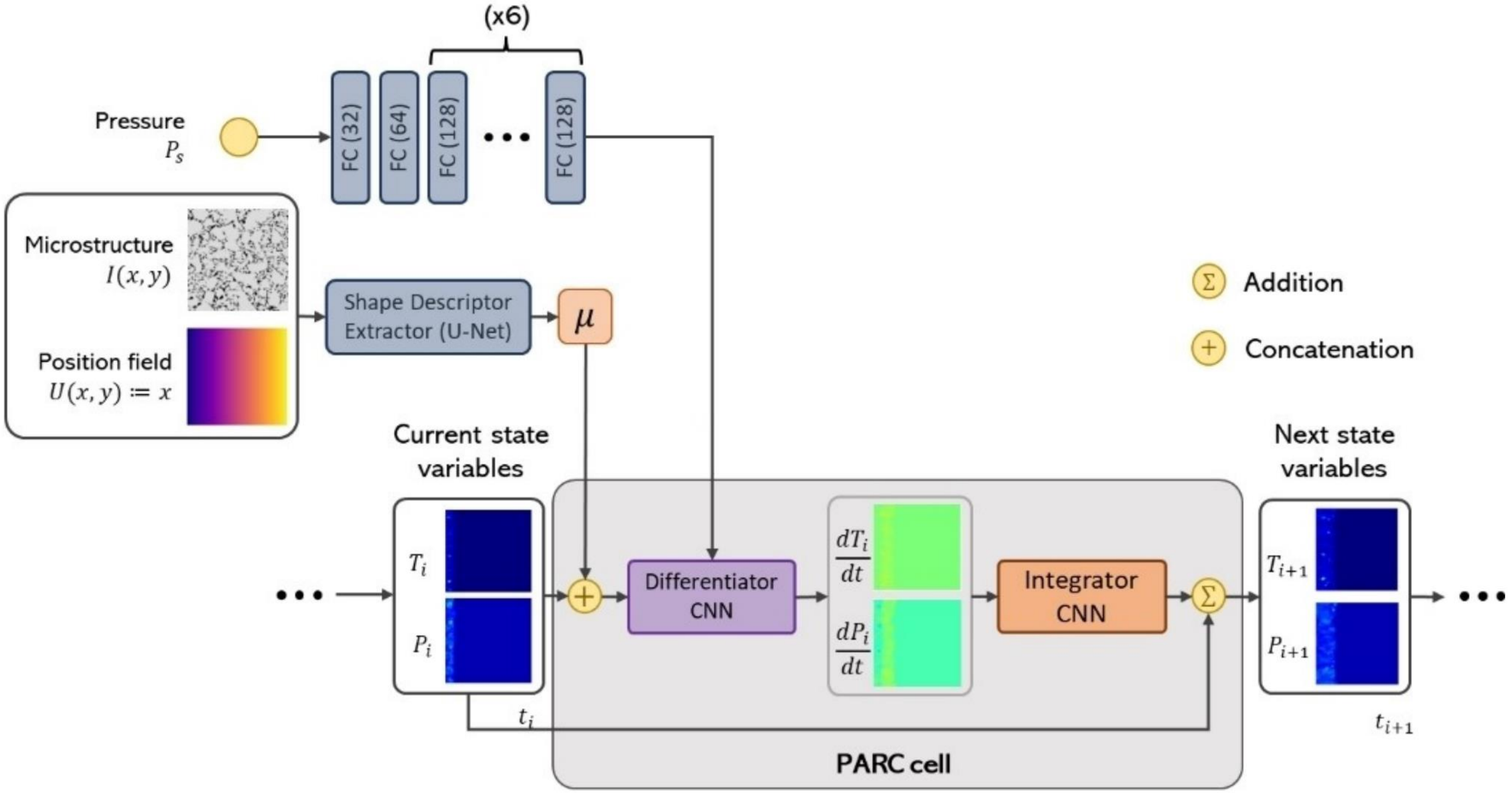
$$\mathrm{AdaIN}(\mathbf{x}_i, \mathbf{y}) = \mathbf{y}_{s,i} \frac{\mathbf{x}_i - \mu(\mathbf{x}_i)}{\sigma(\mathbf{x}_i)} + \mathbf{y}_{b,i},$$

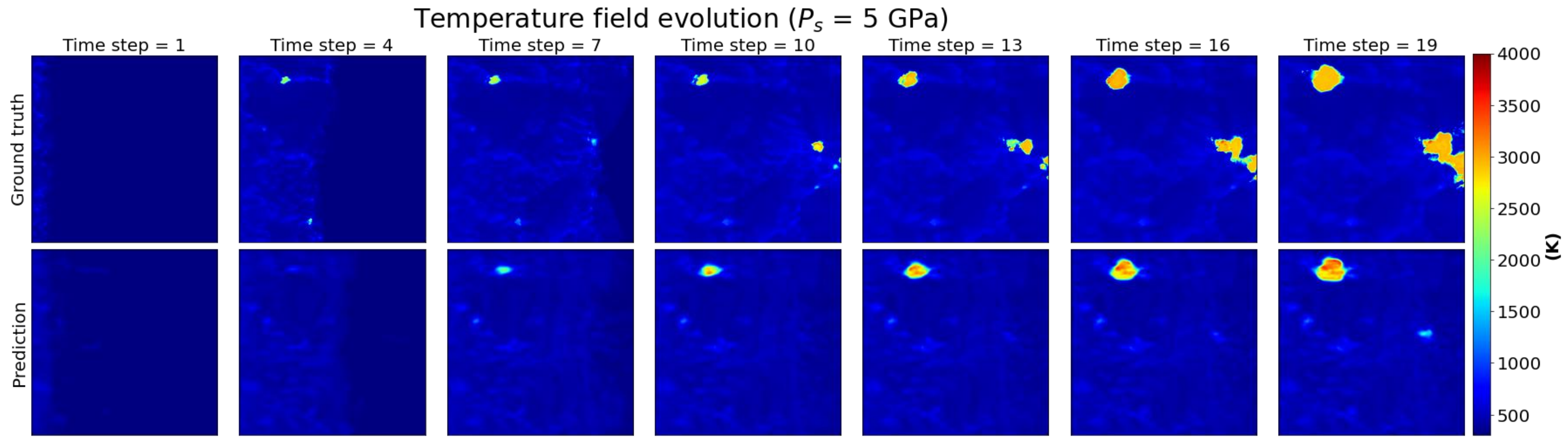
Karras, Laine, & Aila. "A Style-Based Generator Architecture for Generative Adversarial Networks," CVPR 2019

Introducing "Bias" to represent the effects of different shock loadings.

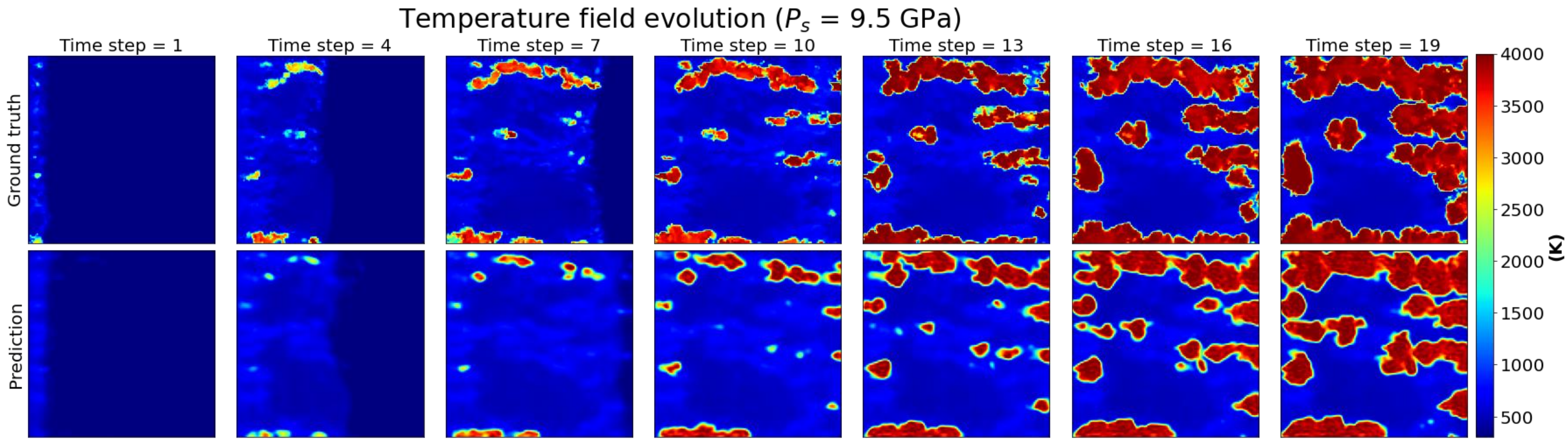


PARCel – Extending PARC to other operating conditions





Nguyen et al. (2023). https://doi.org/10.1002/prep.202200268



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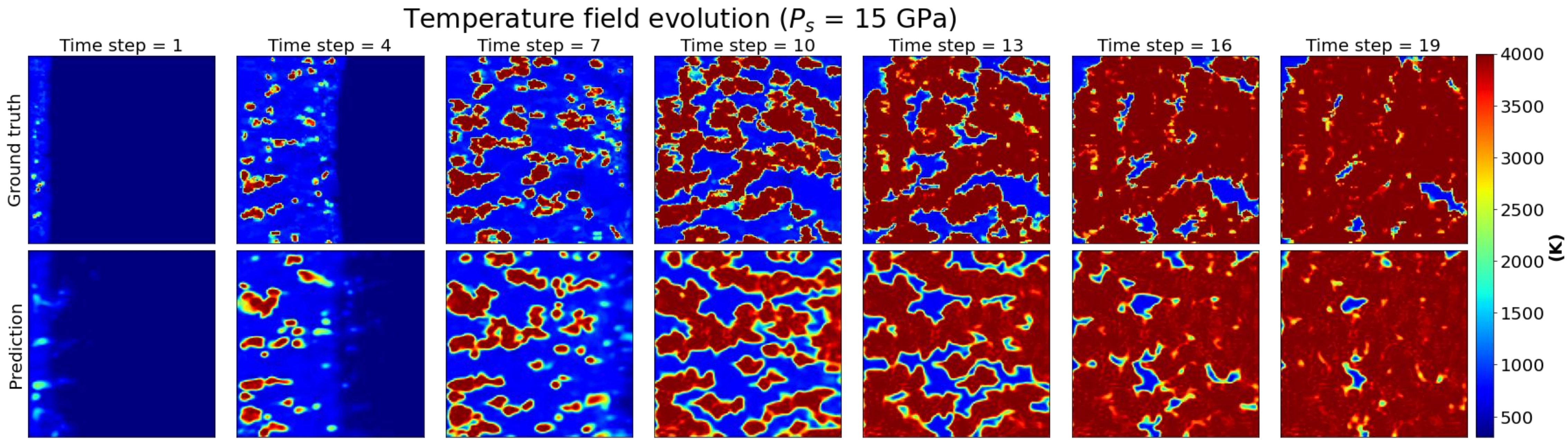
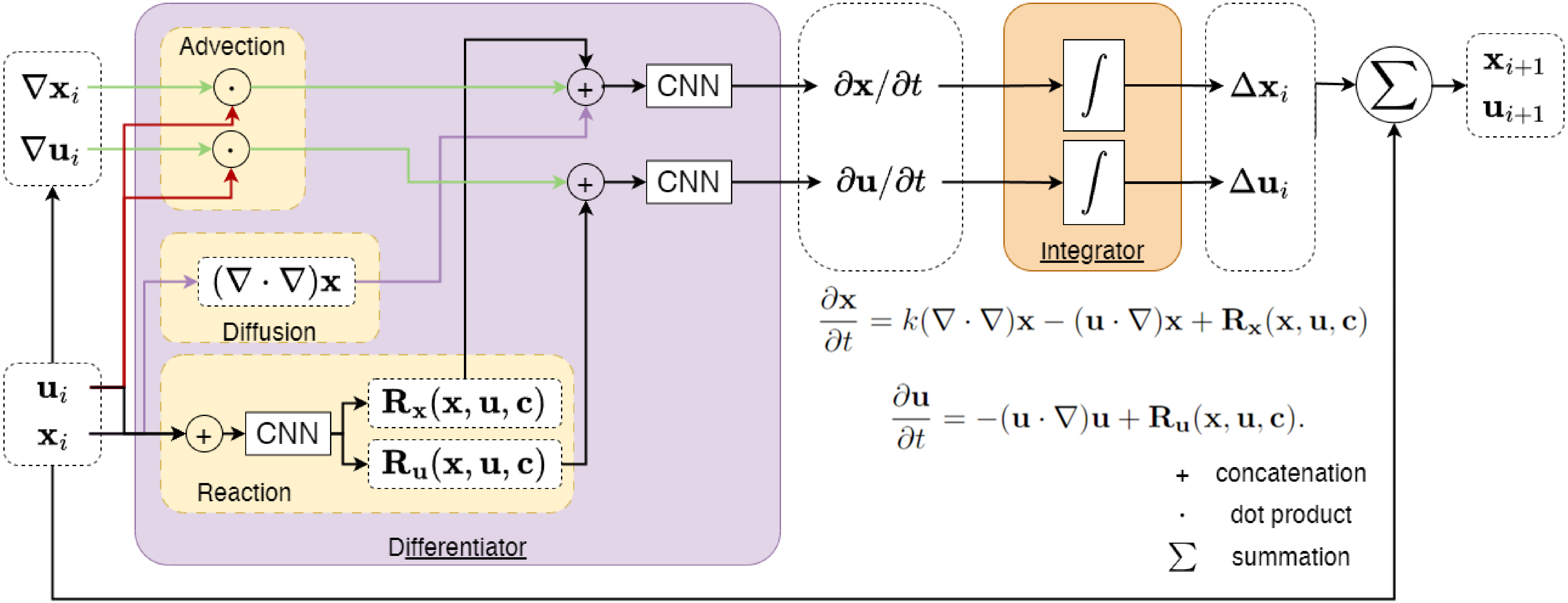


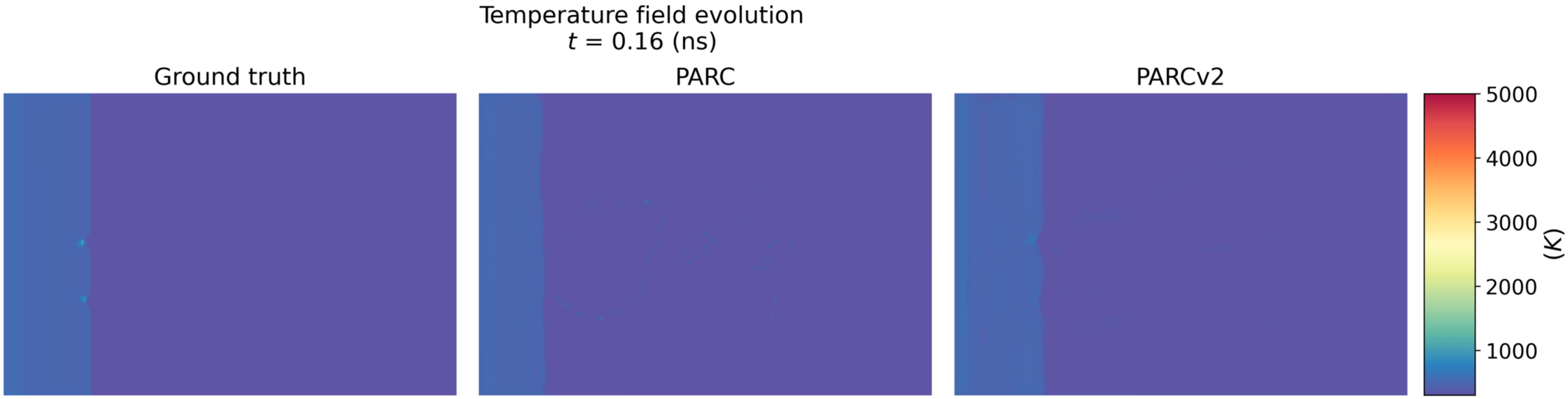
Nguyen et al. (2023). https://doi.org/10.1002/prep.202200268

Physics-Aware Recurrent CNNs (PARCv2)



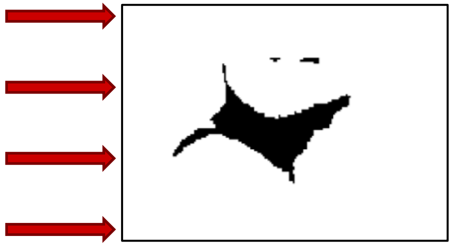
Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

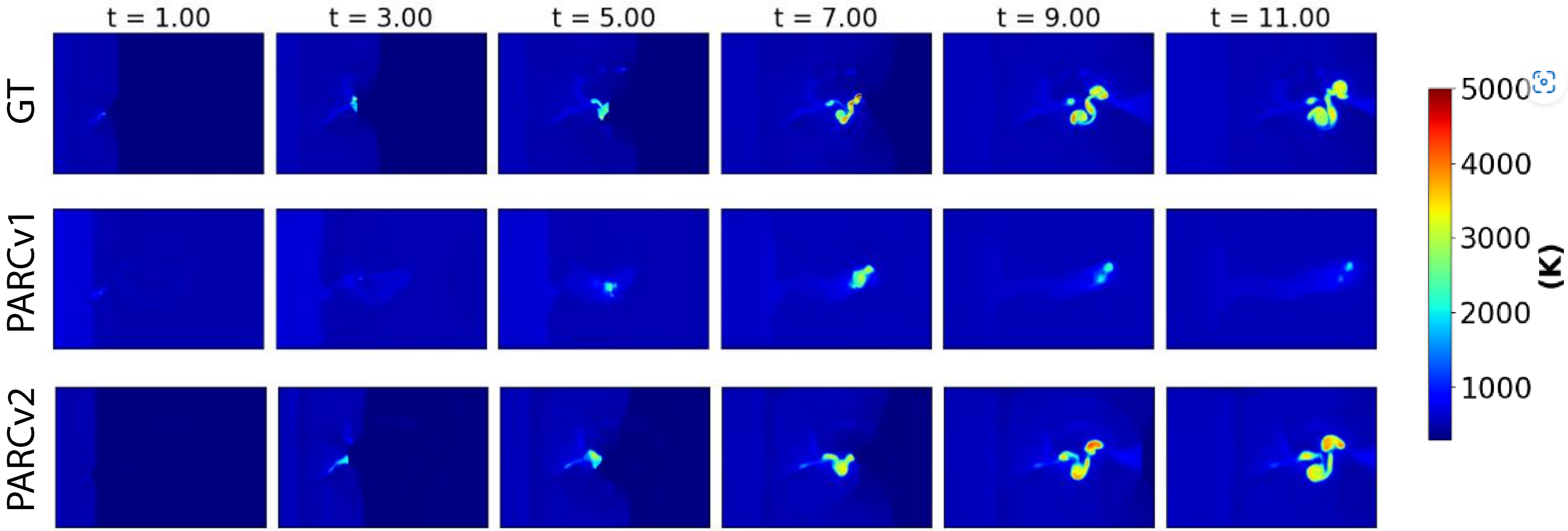
Pore Collapse Simulation



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

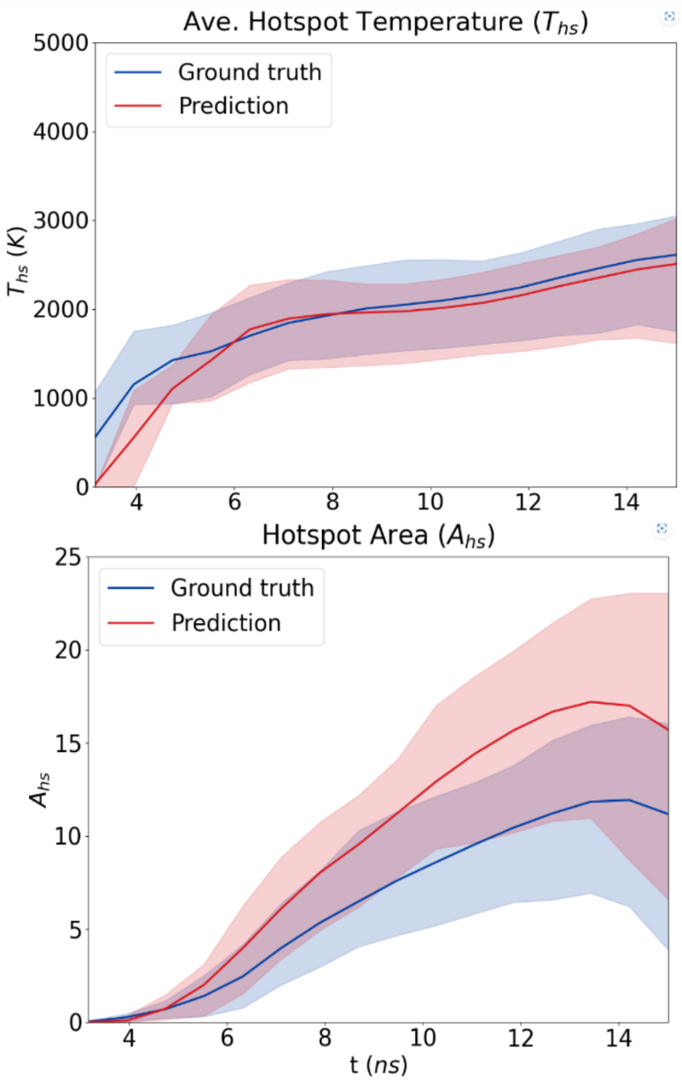
Pore Collapse Simulation

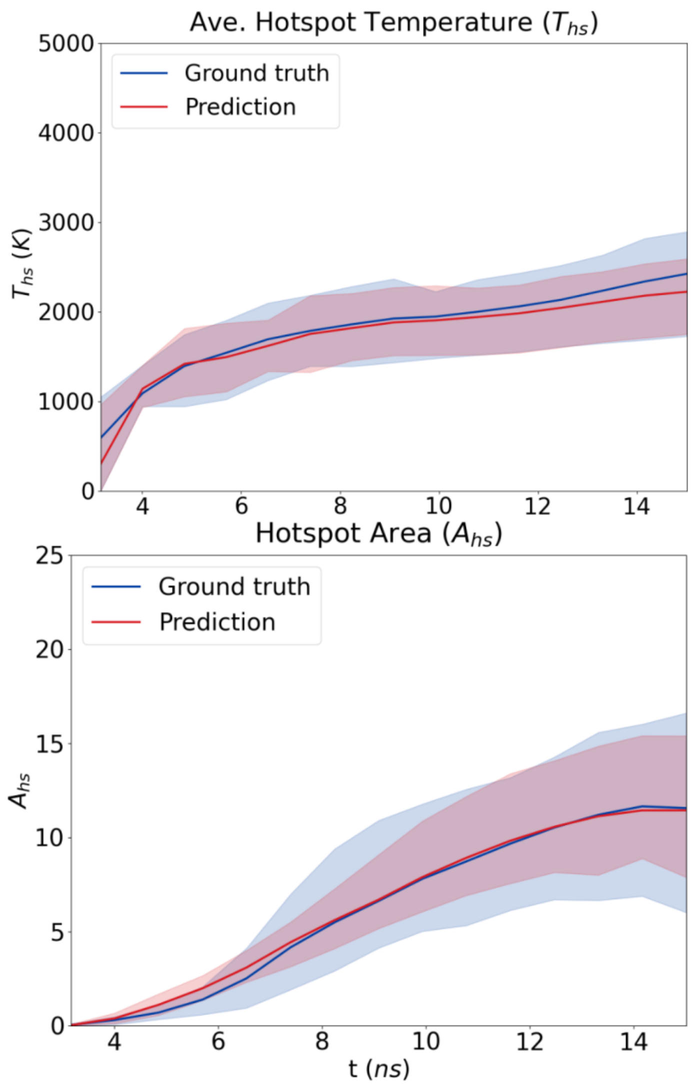




Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

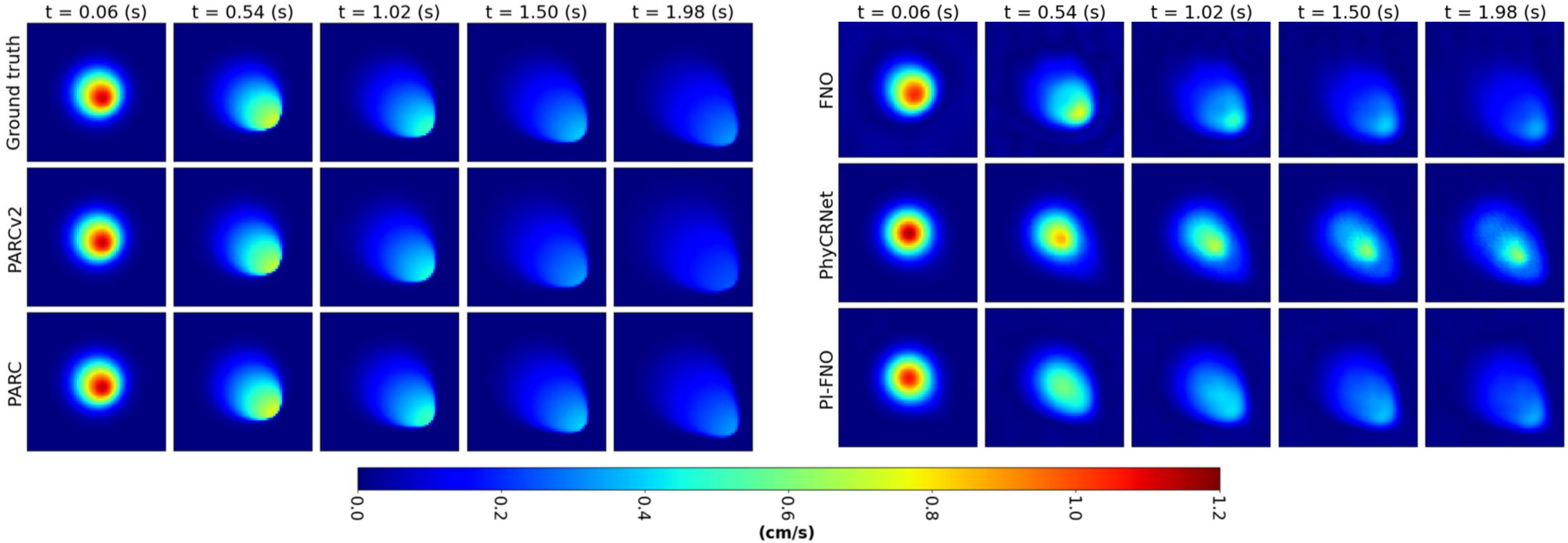
PARCv1 vs. PARCv2





Burgers' Equation

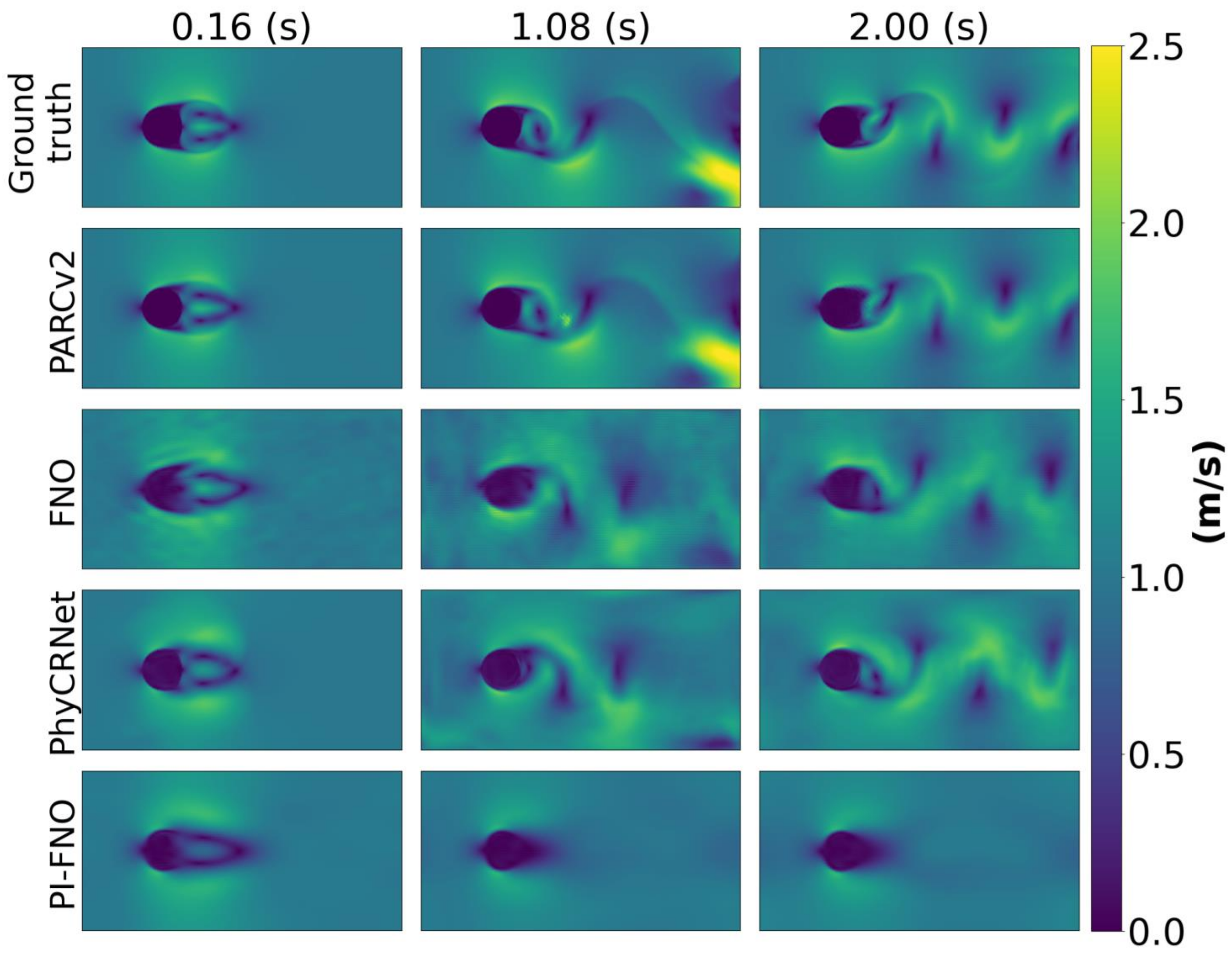
Model	$RMSE_u$ (cm/s)	$\|\|\mathbf{f_u}\|\|$ (cm/s^2)
DNS		0.1241
PARC (numerical int.)	0.0074	0.1262
PARC (data-driven int.)	0.0236	0.1176
FNO	0.0289	0.1537
PhyCRNet	0.0588	0.0560
PIFNO	0.0338	0.1058
PARCv2 (This Study)	0.0129	0.1292



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

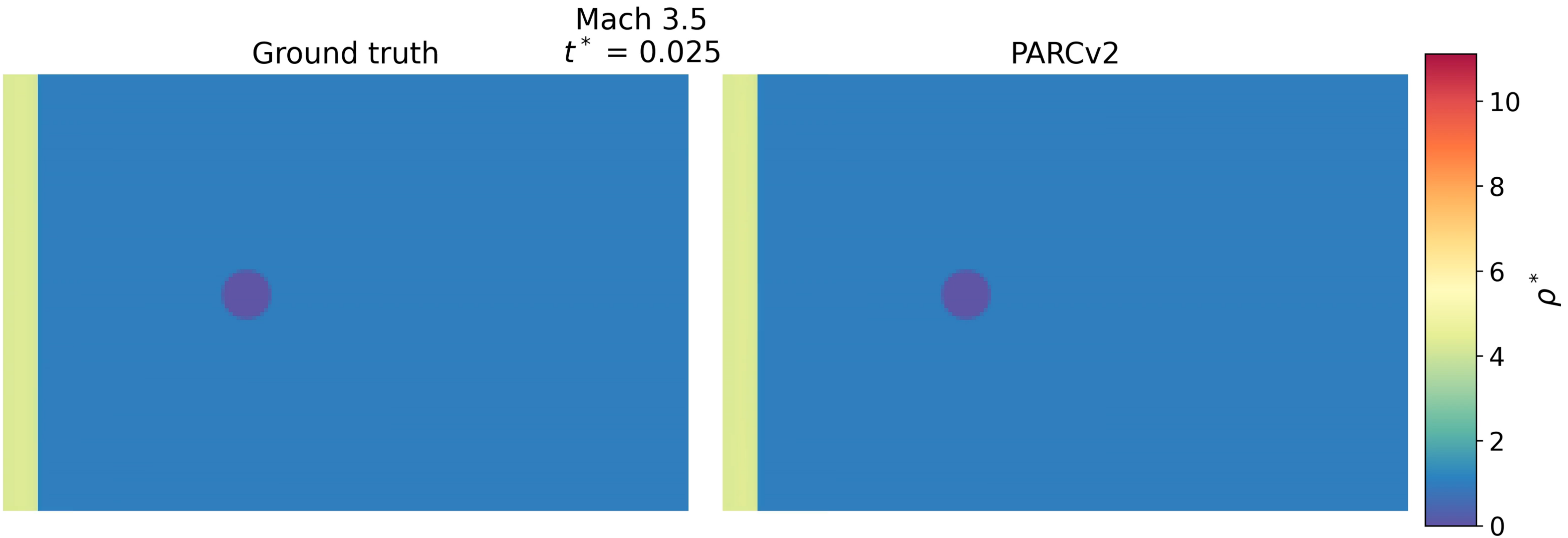
Navier-Stokes Equations

Model	RMSE (cm/s^2)	$\|\|f_{\mathbf{u}}\|\|$ (m/s^2)	ε_{div} $(1/s)$
DNS (Ground truth)	-	2.2339	0.0198
FNO	0.2411	3.2804	1.0471
PhyCRNet	0.2324	2.6994	0.0597
PI-FNO	0.2230	1.4488	0.0307
PARCv2	0.1556	3.0402	0.3655



Nguyen et al. (2024). https://arxiv.org/abs/2402.12503

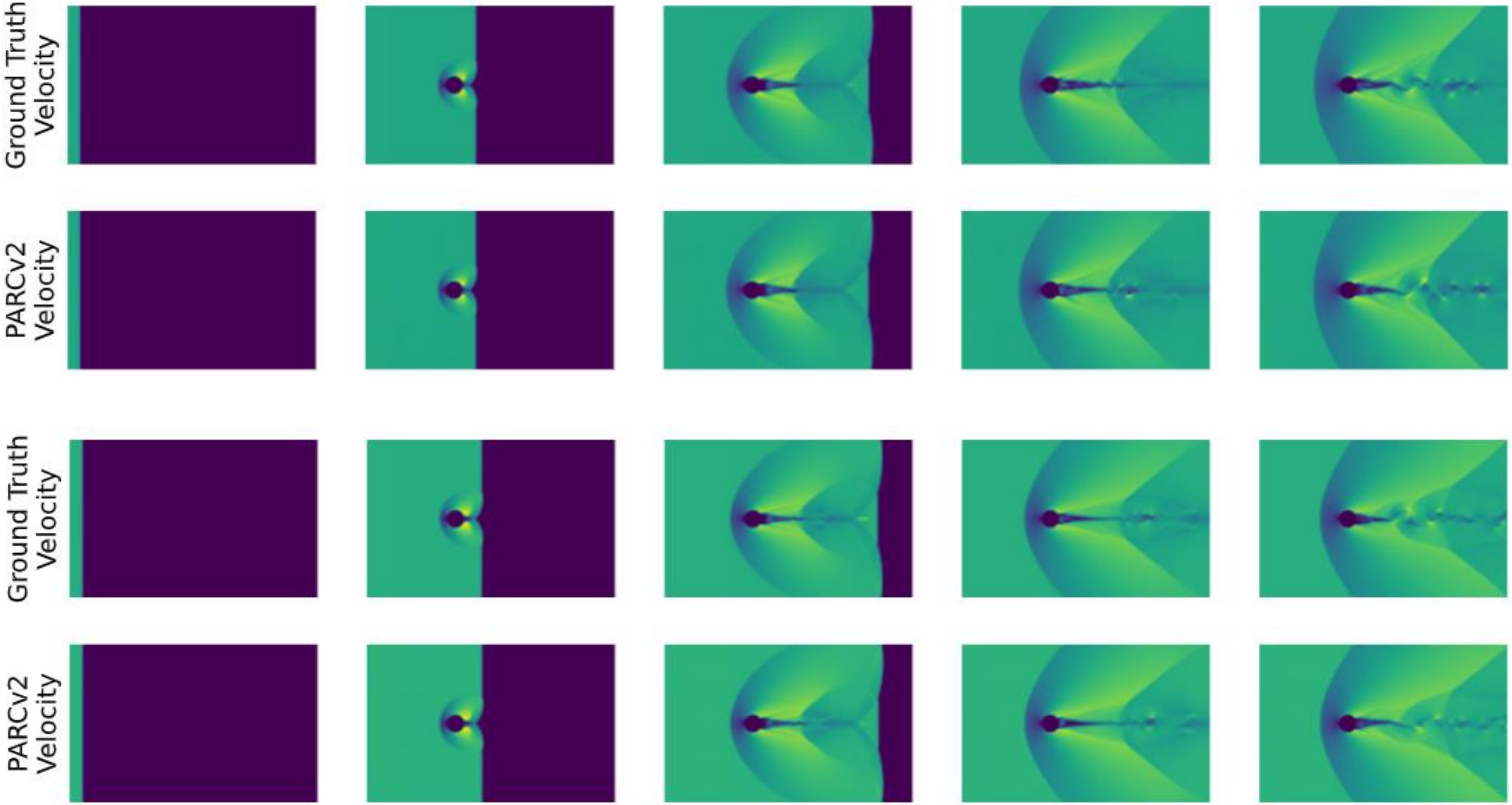
Compressible, Supersonic Flow



Compressible, Supersonic Flow

Mach 3

Mach 4



Summary

- PARC features its “differentiator-integrator architecture” mimicking how PDEs are solved in physics-based solvers
- Comparable accuracy & fidelity to DNS, but multiple orders of magnitude faster (hours on an HPC versus less than a second on a laptop)
- Tends to capture sharp gradients & fast transients better, compared to other physics-informed models.