# Message Passing is all you need!

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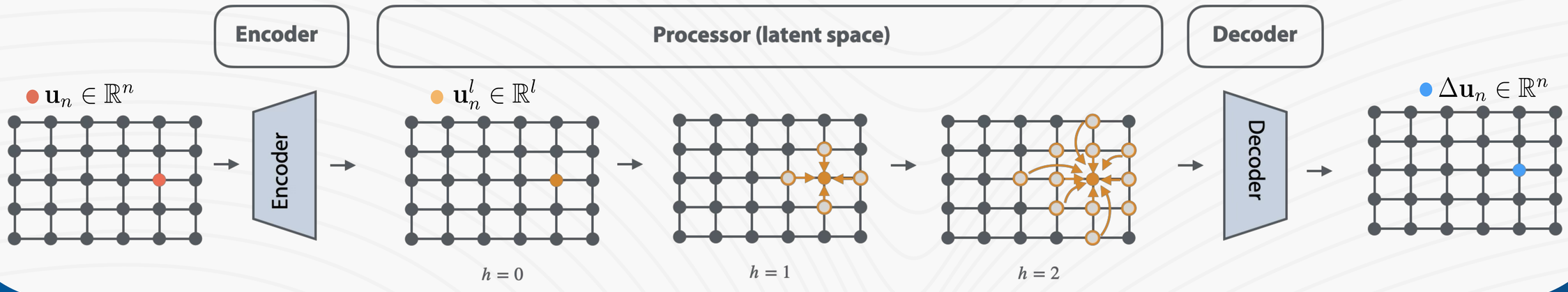
## Graph Neural Networks

### Simulating PDEs with AI?

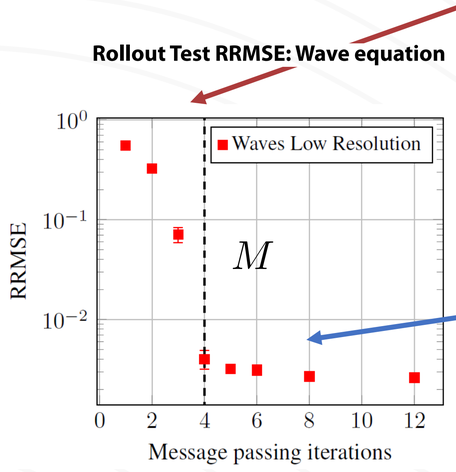
**Explicit Scheme:** $\Delta \mathbf{u}_n = \mathrm{GNN}(\mathbf{u}_n, \boldsymbol{\theta})$, $\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta \mathbf{u}_n$,

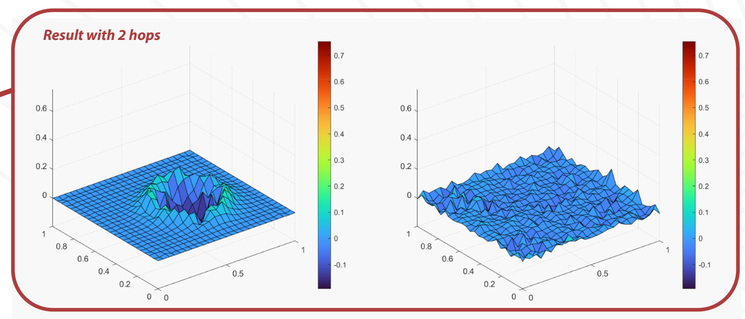
**Node processor - Message aggregation:** $\boldsymbol{\xi}_i^{h+1} = \varphi\left(\boldsymbol{\xi}_i^h, \sum_{j \in \mathcal{N}(i)} \boldsymbol{\xi}_j^h, \boldsymbol{\theta}\right)$

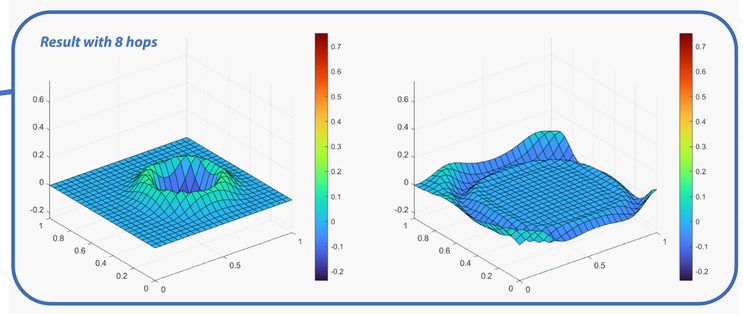



# How many message passes must we do?

## Phenomena governed by hyperbolic equations



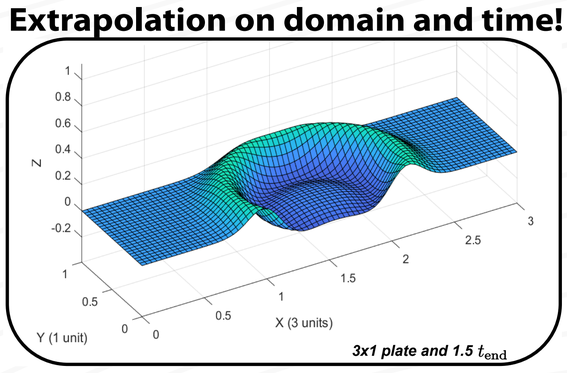




$$\frac{\partial^2 u}{\partial t^2} = c^2 \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = c^2 \nabla^2 u, \qquad M > \sqrt{2} \frac{c \Delta t}{\Delta x}$$

! If we model an hyperbolic system with a GNN **the wave propagation cannot exceed the message transmission distance** in any time increment. **This limit is designated as *M*.**

**But once satisfied...**

**Extrapolation on domain and time!**




## Phenomena governed by parabolic and elliptic PDEs

! Convergence requires **global information propagation** across the domain.

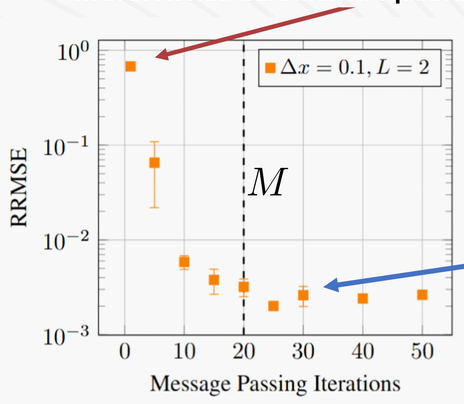
$$M = \frac{L}{\Delta x}$$

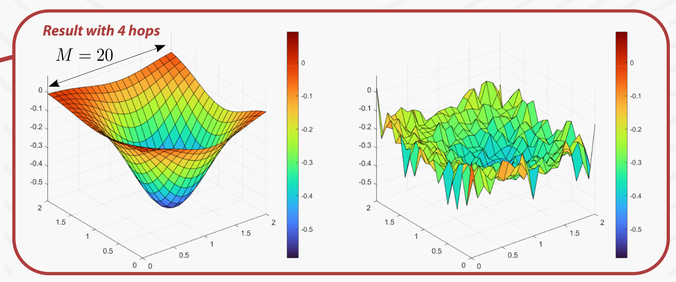
where L denotes the size of the domain, Δx is the spatial discretization.

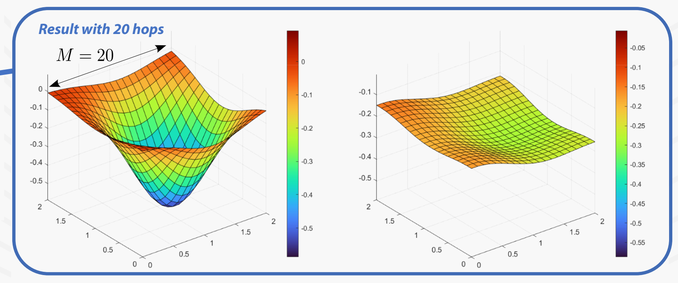
**Thermal Diffusion Equation**

$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u \quad \text{in } \Omega \times (0, T]$$

**Rollout Test RRMSE: Diffusion equation**



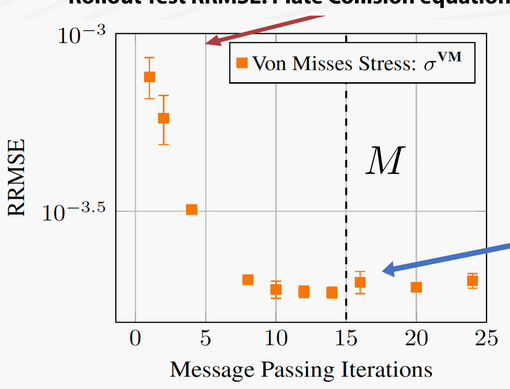



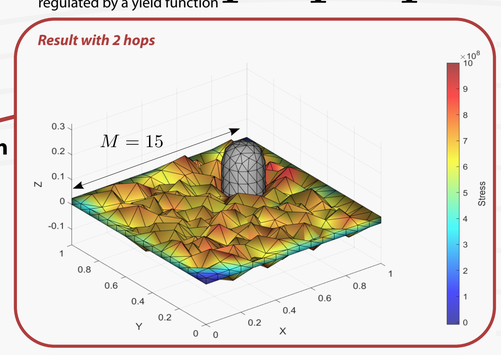

**Incremental Forming**

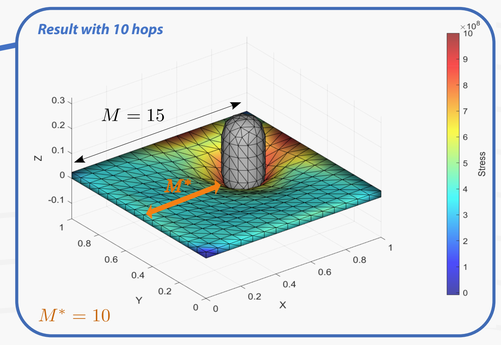
$$\nabla_0 \boldsymbol{P} + \boldsymbol{f}_0 = \boldsymbol{0}, \qquad \boldsymbol{F} = \boldsymbol{F}^{el} \cdot \boldsymbol{F}^{pl}$$

regulated by a yield function

**Rollout Test RRMSE: Plate Collision equation**




## References

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Funded by the European Union NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
GOBIERNO DE ESPAÑA MINISTERIO PARA LA TRANSFORMACIÓN DIGITAL Y DE LA FUNCIÓN PÚBLICA
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