



*Exceptional service in the national interest*



# ACCELERATING MATERIALS SIMULATIONS WITH ML: ROB PETER TO PAY PAUL?



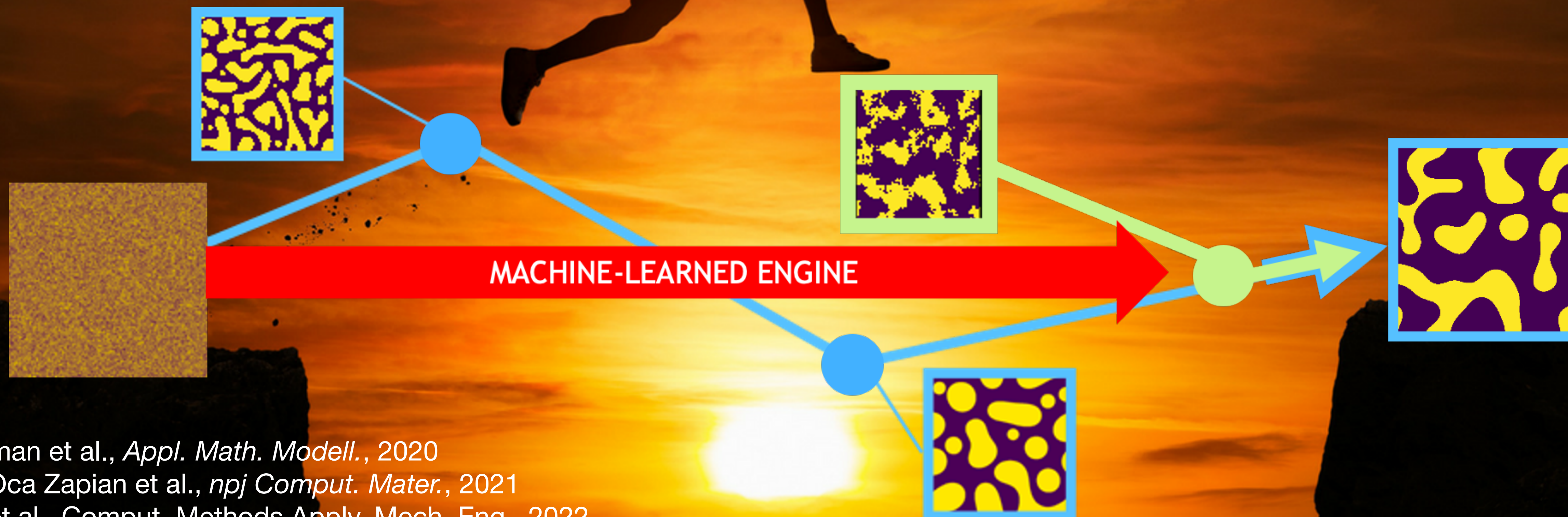
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● → High-fidelity phase field trajectory

● → Accelerated trajectory

- POLYNOMIAL CHAOS EXPANSION
- RNNs
- DEEPONET



Herman et al., *Appl. Math. Modell.*, 2020  
De Oca Zapian et al., *npj Comput. Mater.*, 2021  
Hu et al., *Comput. Methods Apply. Mech. Eng.*, 2022  
Oommen et al., *npj Comput. Mater.*, 2022



WE HAVE NOT SUCCEEDED YET!

**SPEEDING UP THE  
LEARNING WORKFLOW**



**USEFUL  
(SPATIO-TEMPORAL )  
REPRESENTATIONS**

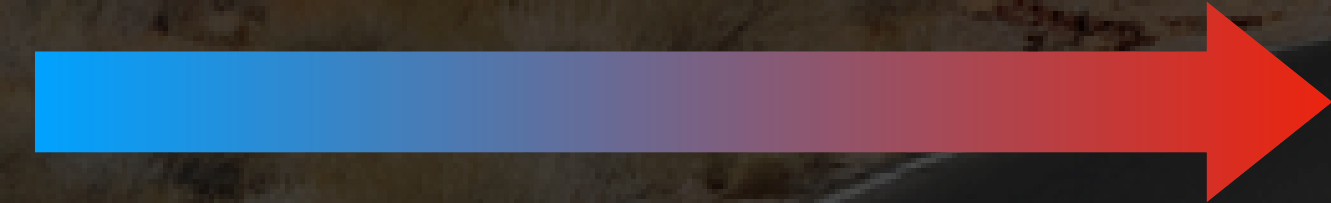


**TOWARDS  
REAL DATA FUSION**



SMALL DATA

BIG DATA



LOT OF  
PHYSICS

NO PHYSICS

