Physics-Aware AI-Directed Framework for Microstructural Design of Shocked Materials

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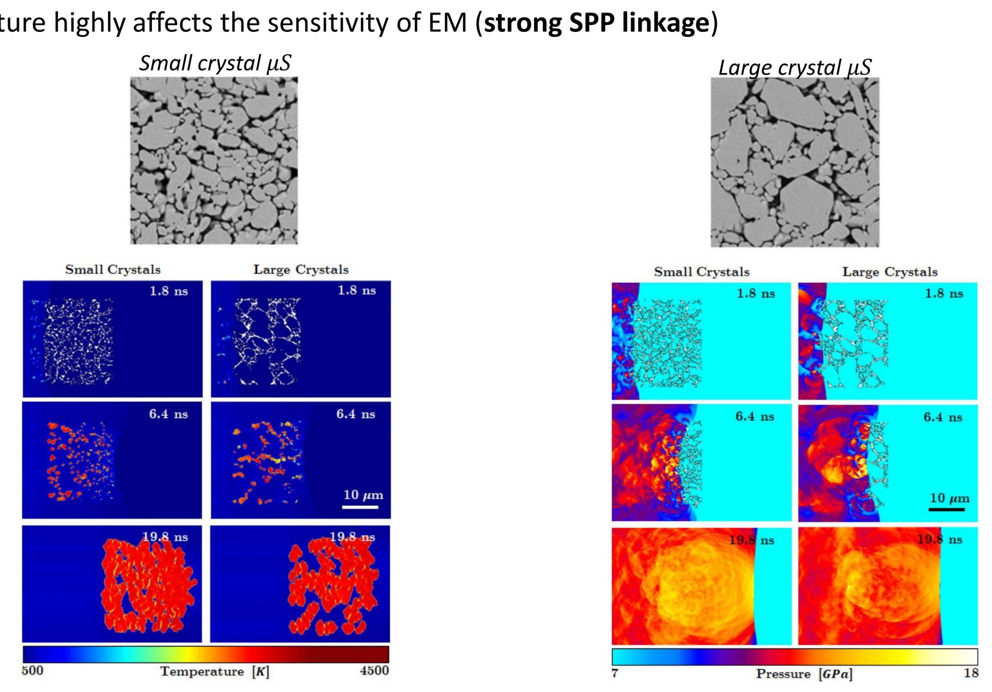
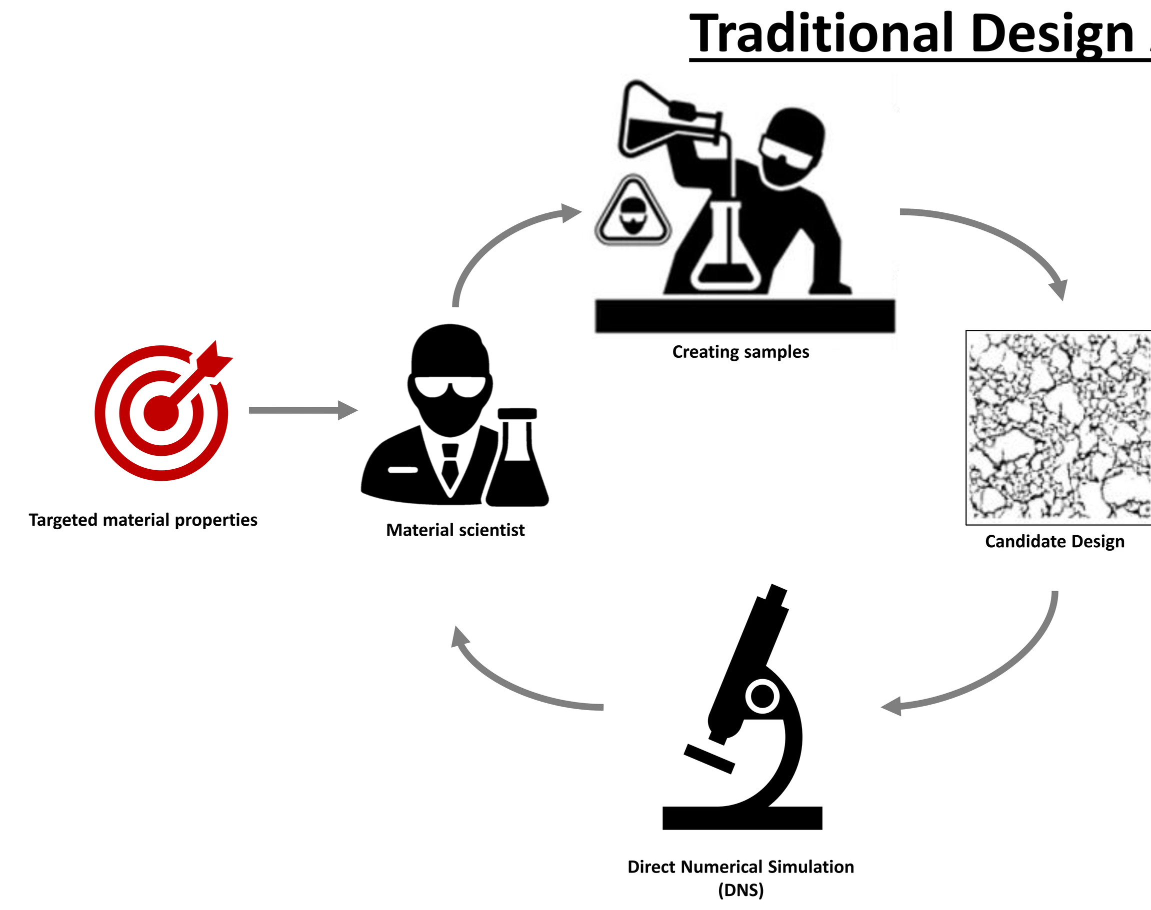
UVA DATA SCIENCE

Pressed Energetic Material (EM) and its background

- **Key component in many applications** (propellant, mining)
- **Sensitivity** (performance and safety)
- Microstructure highly affects the sensitivity of EM (**strong SPP linkage**)



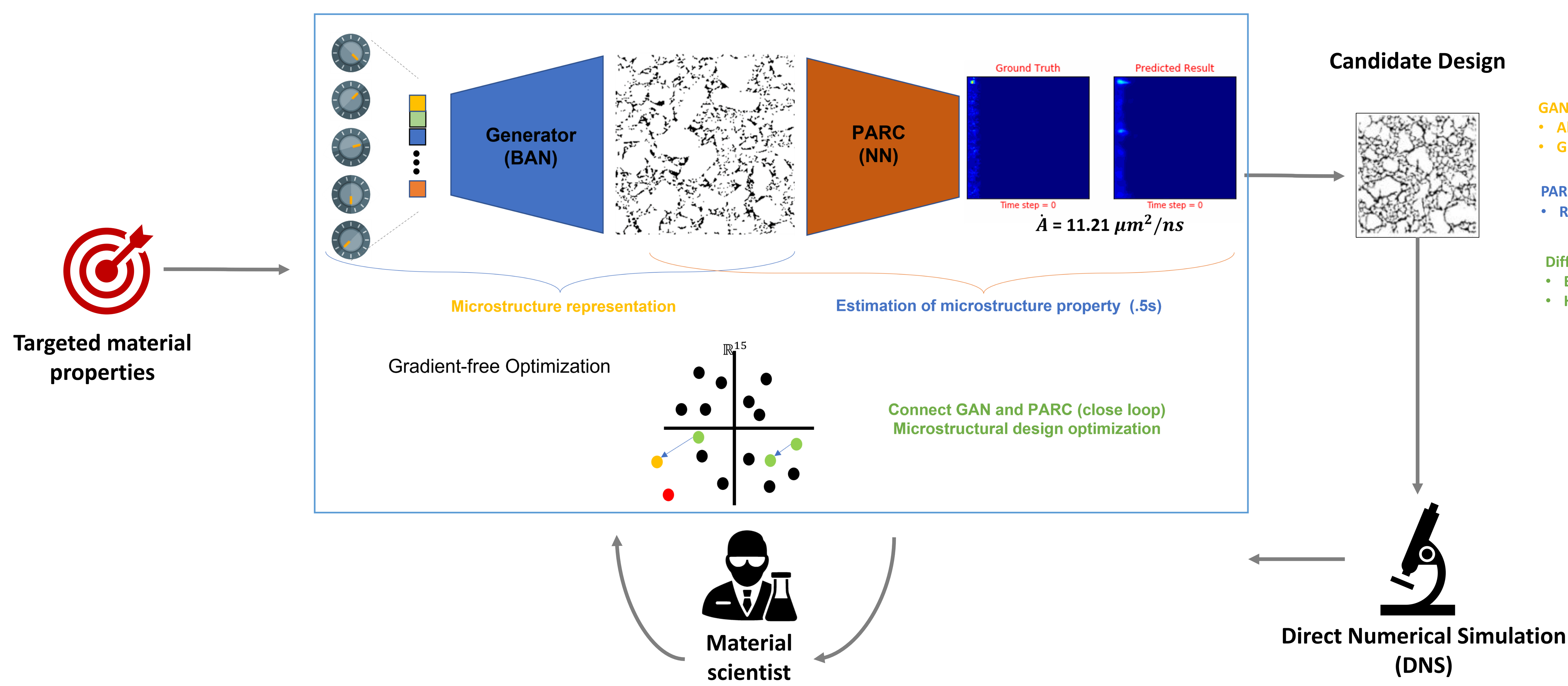
Traditional Design Approach



- **Slow and expensive** (hours - days)
- **Vast search space**
- **Limited (idealized) representation**
  - Geometric primitives
    Simple shape descriptors
  - Not able to model all complex microstructure detail

Practically impossible to fully explore the design space and converge on an optimal solution

Suggested Framework



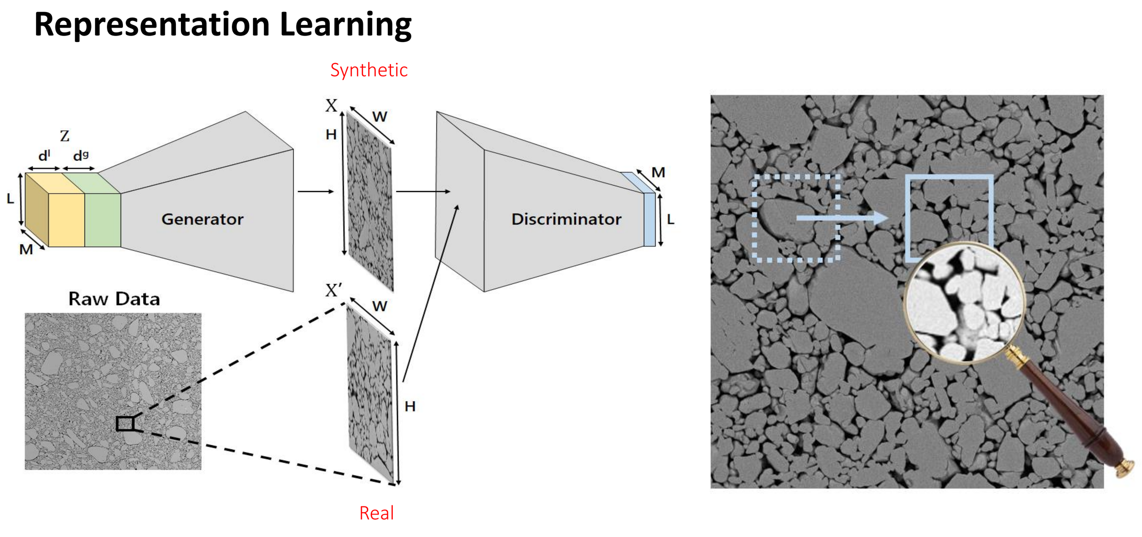
GAN
- All possible shapes and configurations represented
- Great controllability

PARC
- Rapid and accurate estimation of $\dot{A}$ ($\sim .5s$)

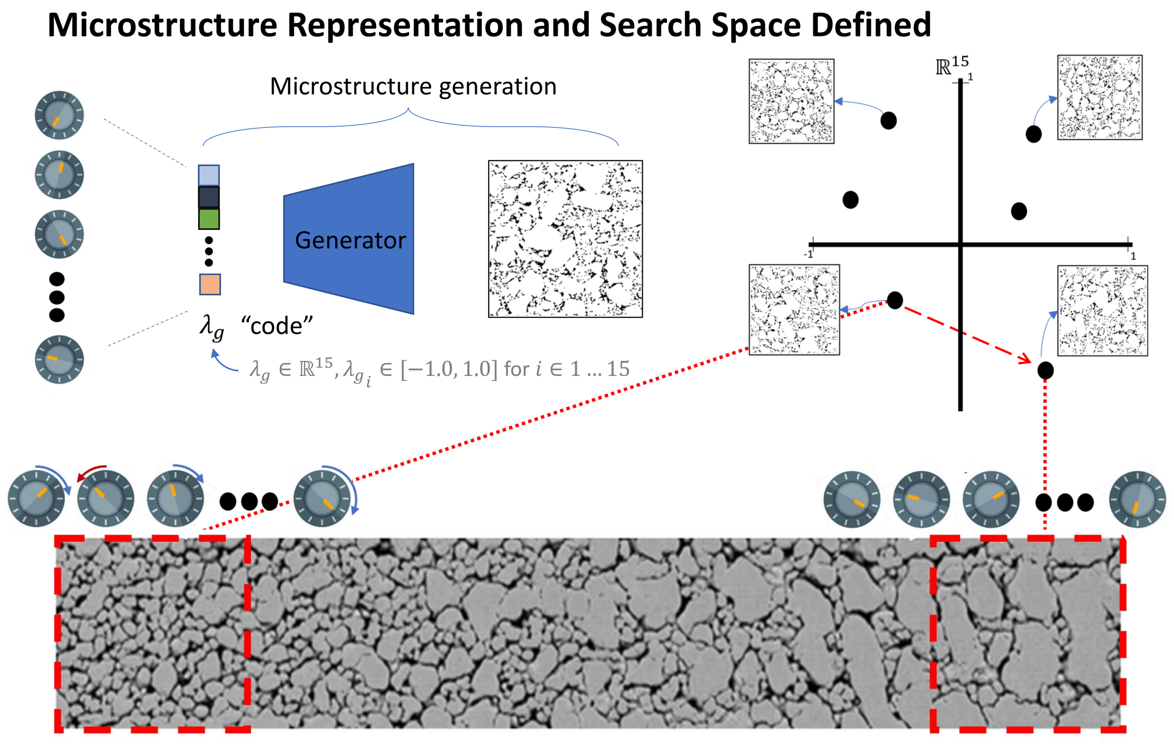
Differential Evolution with Expected Improvement
- Efficient (speed)
- High-quality suggestion

Generative Adversarial Network (GAN)

Representation Learning



Microstructure Representation and Search Space Defined



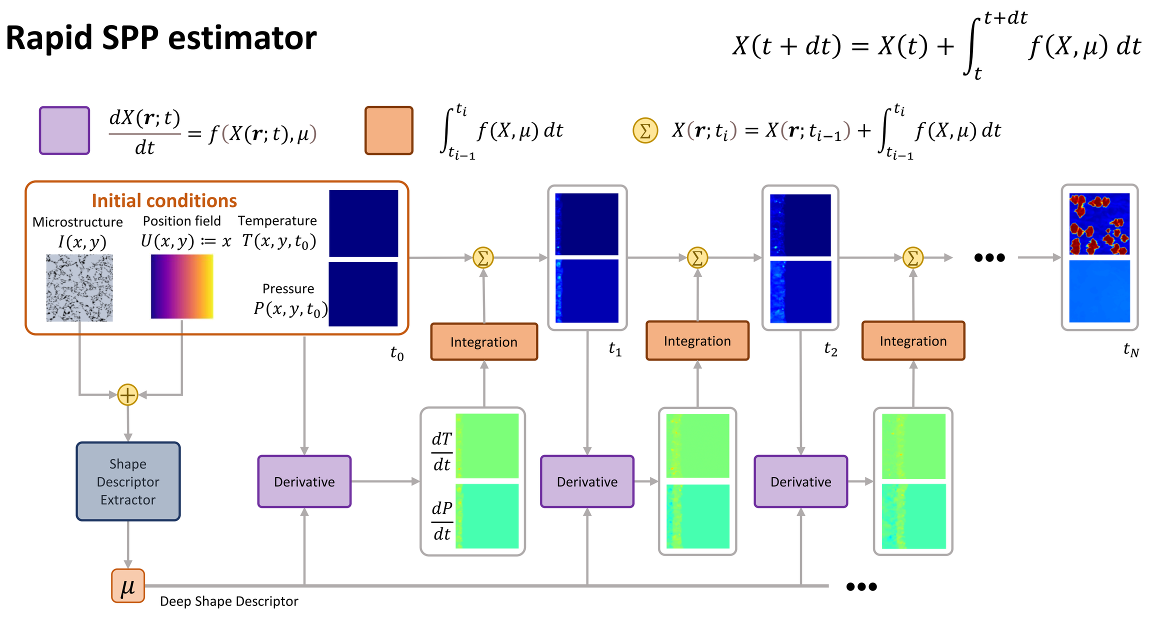
Result
- **Strong Parameterization:**
  parameterize microstructural design with low-dimensional latent vector
- **Controllability**
  allows sophisticated optimization

Chun et al. (2020). Deep learning for synthetic microstructure generation in a materials-by-design framework for heterogeneous energetic materials. *Sci Rep* **10**, 13307 (2020).

Physics-Aware Recurrent Convolution (PARC)

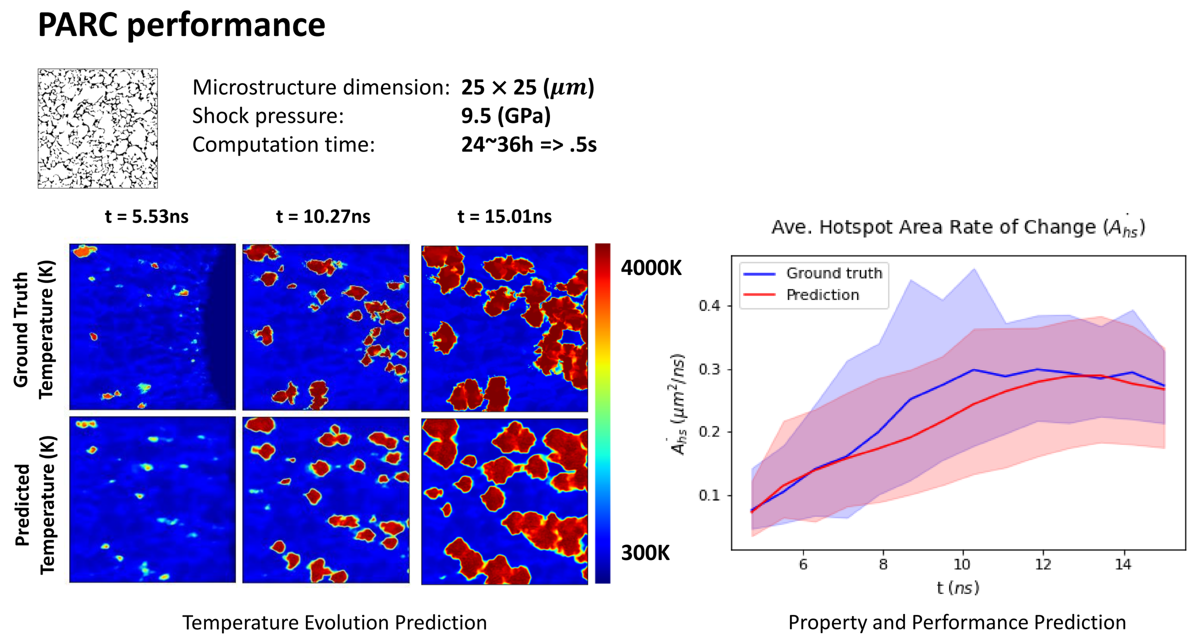
Rapid SPP estimator

$$X(t+dt) = X(t) + \int_t^{t+dt} f(X,\mu)\,dt$$



PARC performance

Microstructure dimension: **25 × 25 (μm)**
Shock pressure: **9.5 (GPa)**
Computation time: **24~36h => .5s**



Temperature Evolution Prediction

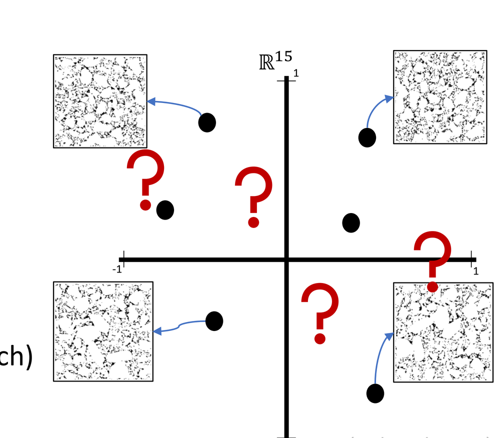
Property and Performance Prediction

Result
- **Rapid SPP estimation:**
  from 24 ~ 48 hours to 0.5 seconds in a commodity desktop
- **Interpretable and Accurate estimation**
  PARC was carefully designed to model differential equations of thermodynamics of energetic materials.

Nguyen, et al. (2022). Physics-Aware Recurrent Convolutional (PARC) Neural Networks to assimilate meso-scale reactive mechanics of energetic materials. *arxiv:2204:07234.*

Differential Evolution with EI

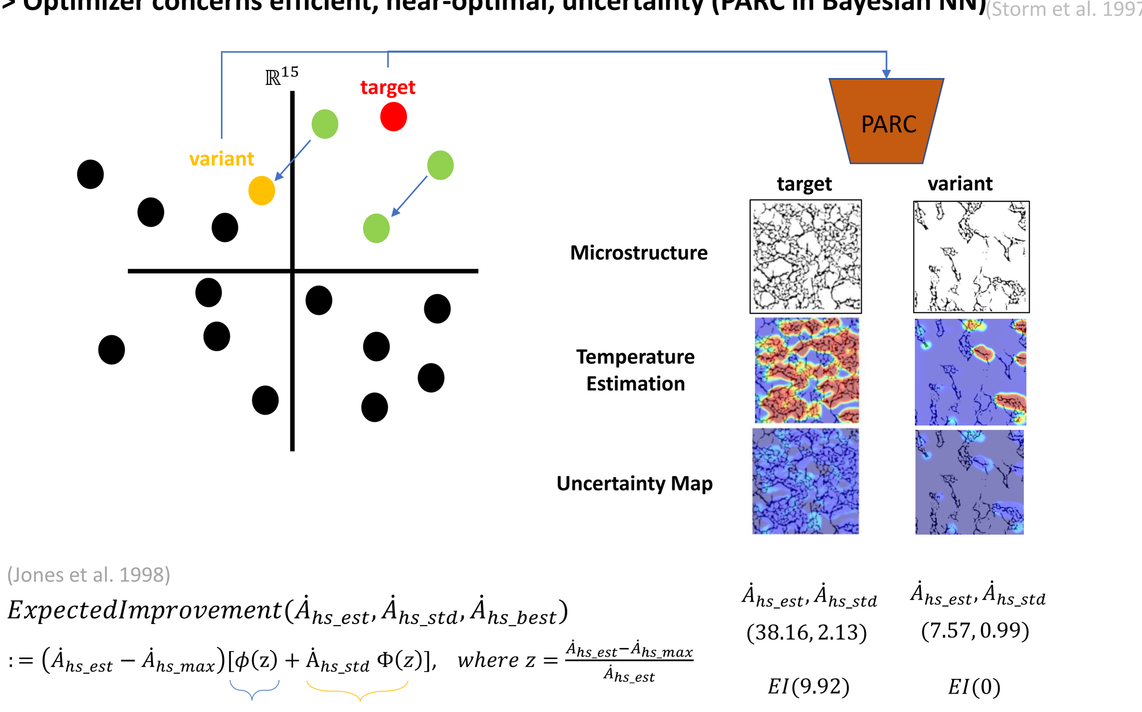
Microstructure Design Optimization



AI-assistants
- GAN Microstructure Representation (search space)
- PARC Rapid and accurate estimation (<1s)

Challenges
- Complex Objective function (latent space)
- Vast Search Space (10^6 evals. for grid search)
- Scarce Labeled data (prone to overfitting)

=> Optimizer concerns efficient, near-optimal, uncertainty (PARC in Bayesian NN) (Gal et al. 2015) (Storn et al. 1997)



(Jones et al. 1998)

$$ExpectedImprovement(\dot{A}_{hs\_est}, \dot{A}_{hs\_std}, \dot{A}_{hs\_best})$$
$$:= (\dot{A}_{hs\_est} - \dot{A}_{hs\_max})[\phi(z) + \dot{A}_{hs\_std}\,\Phi(z)], \quad where\ z = \frac{\dot{A}_{hs\_est} - \dot{A}_{hs\_max}}{\dot{A}_{hs\_est}}$$

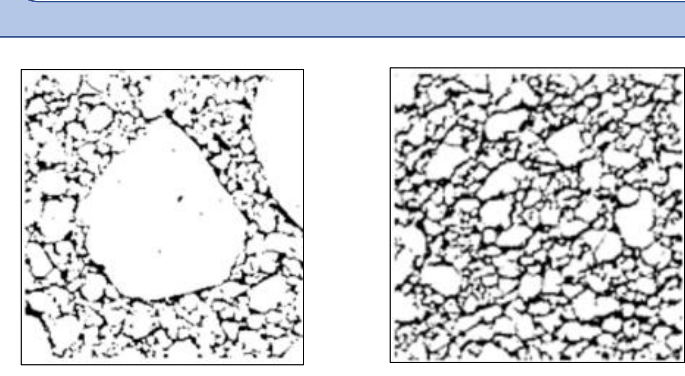
Exploitation: Strive for best $\dot{A}_{hs}$ on **current knowledge**
Exploration: **Improve knowledge** on uncertain area

Result
- **Efficient, near-optimal solution optimization:**
  A significantly lower number of evaluations, but still provides near-optimal
- **Optimization with uncertainty concerned:**
  Balance in exploitation and exploration using uncertainty from Bayesian PARC

Gal et al. (2015). Dropout as a Bayesian approximation: representing model uncertainty in Deep Learning, In Proc. 33rd Int. Conf. Mach. Learn., pp. 1050–1059.
Storn et al. (1997). Differential Evolution – a simple and efficient heuristic for global optimization over continuous spaces. Journal of Global Optimization 11, 341-359.
Jones et al. (1998). Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13(4):455-492.

Experiments and Results

- 42 cases of HMX with the initially best reaction rate of 28.23 $\mu m^2/ns$
- Found new microstructural design with **over 180% increase** (53.18 $\mu m^2/ns$)
- Voids mostly **aligned parallel to the direction of the shock propagation** are highly reactive



Previously best known **Newly discovered**

Conclusion

- Suggested AI-assisted framework for microstructural design with targeted property:
  1) GAN: for better microstructure representation (search space)
  2) Bayesian PARC: for accurate and rapid estimation (from 24-36 hours to 0.5s)
  3) Efficient Optimizer: gradient-free optimization with uncertainty (efficient, near optimal
- Validated suggested framework by discovering microstructural design with over 180% increase in reaction rate