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Genetic programming for interpretable, data-driven continuum damage models

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Abstract

- Mechanisms of ductile fracture are understood, but constitutive modeling is still difficult.
  - Mechanisms occur at material length scales, but engineering scale analyses are required.
  - Here, the focus is void growth in metals.
- Clever mechanicians have developed quality analytic damage laws in the past.
  - Though effective and efficient, these are limited by necessary assumptions.
- Contemporary computational power enables us to advance.
  - Perform direct numerical simulation (DNS) of explicit microstructural features.
  - Generate large sets of training data to drive machine learning.
  - Obtain a model that captures more of the relevant fine-scale physics.
- Genetic programming with symbolic regression (GPSR) is an attractive option.
  - An analytic damage evolution law: interpretable, simple to integrate in existing workflows.
  - *A data-driven, analytic damage model without making limiting assumptions.*

Outline

- Theoretical background
  - Two existing models for porosity kinetics
  - Genetic programming with symbolic regression (GPSR)
- Calculation strategy
  - Direct numerical simulation (DNS)
  - Data-driven analytic model via GPSR
- Results
  - Comparison with existing model
  - Sandia Fracture Challenge
- Conclusion
- Acknowledgements

Two existing models for porosity kinetics

- Gurson model of porous plasticity
  - Yield surface formulation[1]
    - Possible to cast as damage formulation[2]
  - Focus of our collaborators at Utah and NASA[3]

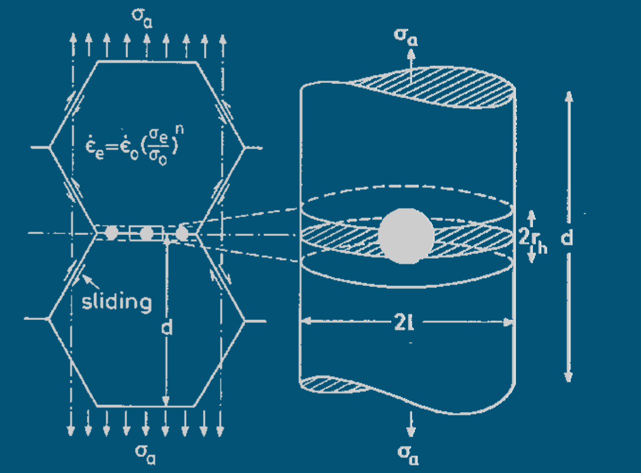
$$\Phi = \left(\frac{\sigma_e}{\sigma_y}\right) + 2\phi \cosh\left(\frac{3\sigma_h}{2\sigma_y}\right) - 1 - \phi^2$$

- Cocks-Ashby model of creep fracture
  - Damage formulation[4]
  - Growth/diffusion of pores on grain boundaries

$$\dot{\phi} = \sqrt{\frac{3}{2}}\,\dot{\epsilon}^p \,\frac{1-(1-\phi)^{n+1}}{(1-\phi)^n}\,\sinh\left[\frac{2(2n-1)}{2n+1}\frac{\sigma_h}{\sigma_e}\right]$$

- Some assumptions of either model (and others)
  - Perfect plasticity or power-law creep
  - Self-similar growth of spherical pores
  - No interaction of pores
  - Isotropic homogeneous matrix

- *Hard to derive analytic models without assumptions, but still possible to obtain them computationally.*

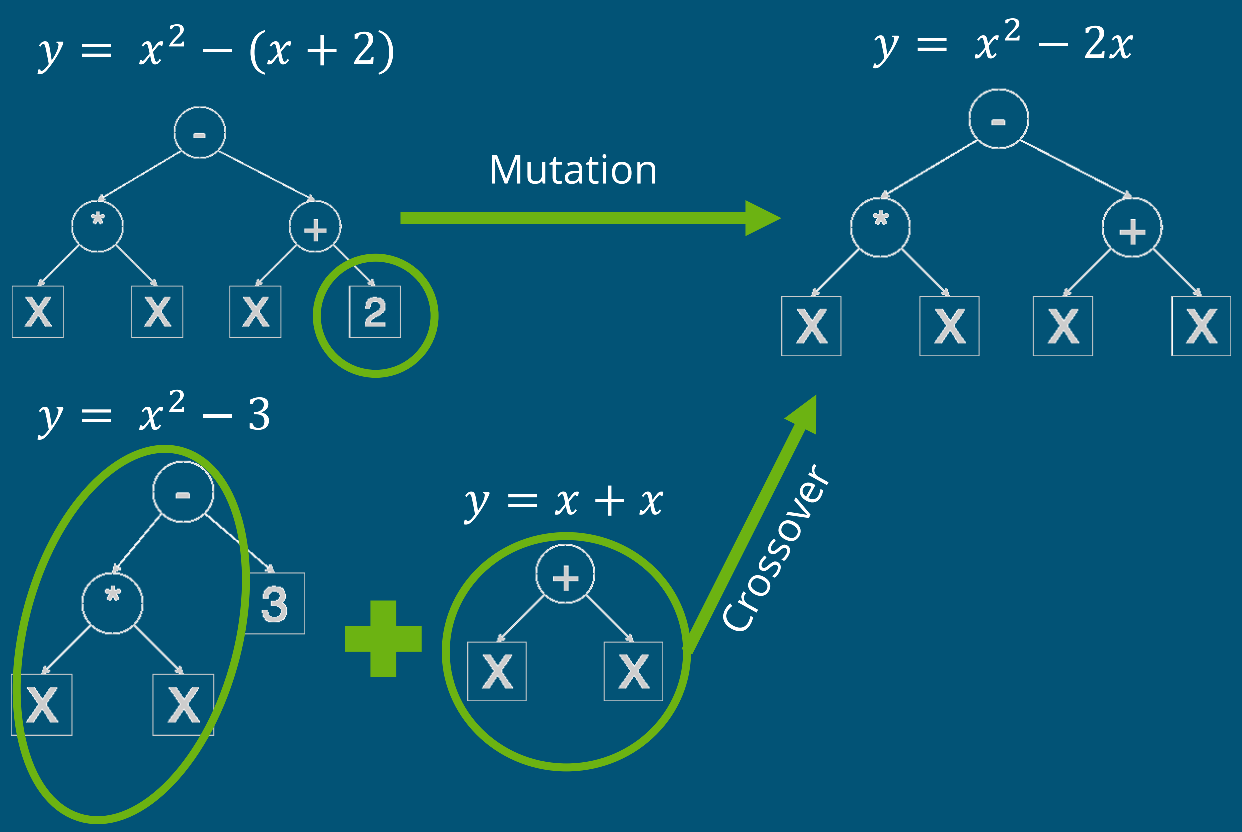


Voids growing on grain boundary in power-law creeping solid

[1] Gurson, A.L. Continuum theory of ductile rupture by void nucleation and growth. *J. Eng. Mater. Technol.* **99**, 2-15 (1977).
[2] Moore, J.A., Frasca, A. A comparison of Gurson and Cocks–Ashby porosity kinetics and degradation functions. *Int J Fract* **229**, 253–268 (2021).
[3] Bomarito, G.F., Townsend, T.S., Stewart, K.M., Esham, K.V., Emery, J.M., Holchhalter, J.D. Development of interpretable, data-driven plasticity models with symbolic regression. *Comp. & Struct.* **252**, 106557 (2021).
[4] Cocks, A.C.F., Ashby, M.F. On creep fracture by void growth. *Prog. in Mater. Sci.* **27**, 189-244 (1982).

Genetic programming with symbolic regression (GPSR)

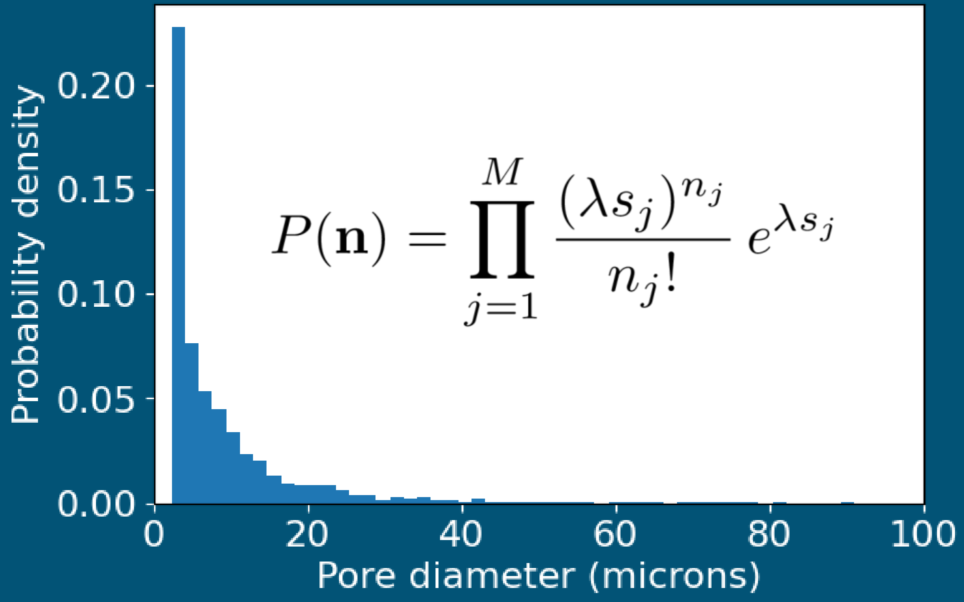
- Genetic programming
  - Evolve models using (data) fitness
- Symbolic regression
  - Combine functions/operations/etc.
  - Implicit or explicit
- Verify models using control data[3]
  - (Verify the GPSR approach)
- Discover models using new data



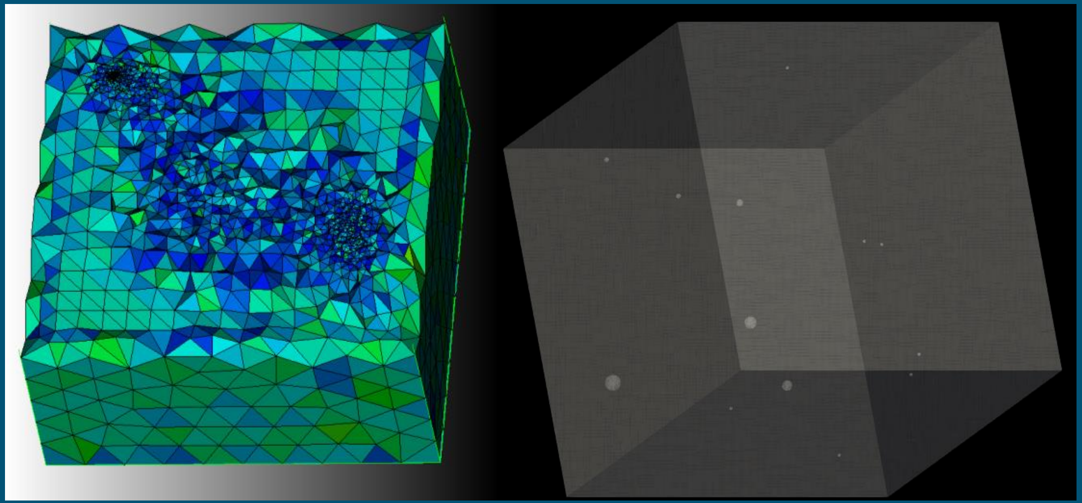
[3] Bomarito, G.F., Townsend, T.S., Stewart, K.M., Esham, K.V., Emery, J.M., Holchhalter, J.D. Development of interpretable, data-driven plasticity models with symbolic regression. *Comp. & Struct.* **252**, 106557 (2021).

Direct numerical simulation (DNS)

- Additively-manufactured 316L stainless steel
  - Porosity data known[5,6] (0.09% porosity; sizes)
- Geometry/mesh using Cubit[7]
  - Poisson point process for pore placement
  - Nominally 10 pores per cube
    - Tractable, convergent meshes
- FE calculations using Sierra[8]
  - Randomly sampled deformations[9]
  - 50 meshes x 50 deformations
  - Von Mises yield, Voce hardening[5]



$$P(\mathbf{n}) = \prod_{j=1}^{M} \frac{(\lambda s_j)^{n_j}}{n_j!} e^{\lambda s_j}$$



[5] Johnson, K.L., et al. Predicting the reliability of an additively-manufactured metal part for the third Sandia fracture challenge by accounting for random material defects. *Int J. Fract.* **218**, 231-243 (2019).
[6] Kramer, S.L.B., et al. The third Sandia fracture challenge: predictions of ductile fracture in additively manufactured metal. *Int J. Fract.* **218**, 5-61 (2019).
[7] Cubit Geometry and Mesh Generation Toolkit, Sandia National Laboratories. U.S. Department of Energy Office of Scientific and Technical Information (osti.gov).
[8] Sierra Solid Mechanics, Sandia National Laboratories. U.S. Department of Energy Office of Scientific and Technical Information (osti.gov).
[9] Fuhg, Jan N., Bouklas, Nikolaos. On physics-informed data-driven isotropic and anisotropic constitutive models through probabilistic machine learning and (...). *Comput. Methods Appl. Mech. Engrg.* **394**, 114915 (2022).

Data-driven analytic model via GPSR

- GPSR using Bingo
  - Open-source software available on GitHub

- Explicit training data:
  - ϕ pore volume fraction (damage)
  - $\dot{\epsilon}^p$ equivalent plastic strain rate $= \sqrt{\frac{2}{3}\dot{\epsilon}^p_{ij}\dot{\epsilon}^p_{ij}}$
  - T triaxiality $= \frac{\sqrt{2}}{3}\frac{\sigma_1+\sigma_2+\sigma_3}{\sqrt{(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2}}$
  - L Lode factor $= \frac{2\sigma_2-\sigma_1-\sigma_3}{\sigma_1-\sigma_3}$

- Obtain Pareto front of models
  - Highest-fitness individuals at each complexity
  - Often best to choose near an “elbow”

github.com/nasa/bingo

$$\dot{\phi} = f(\phi, \dot{\epsilon}^p, T, L)$$

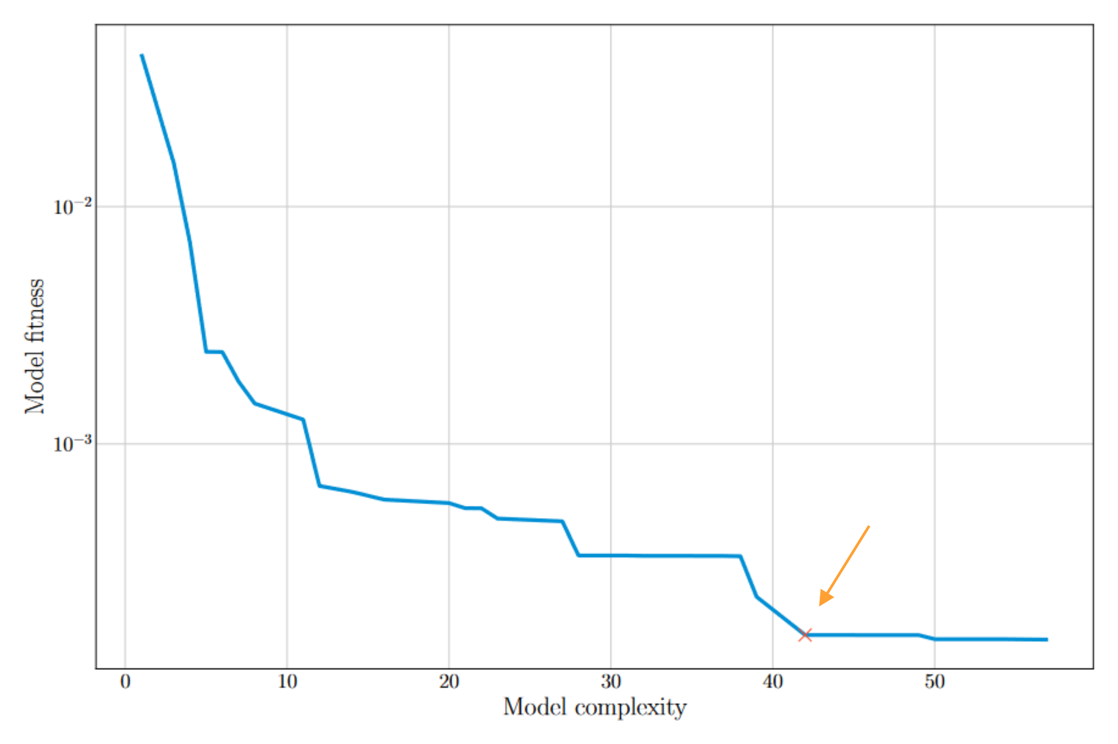
$$\phi \in (0,1)$$

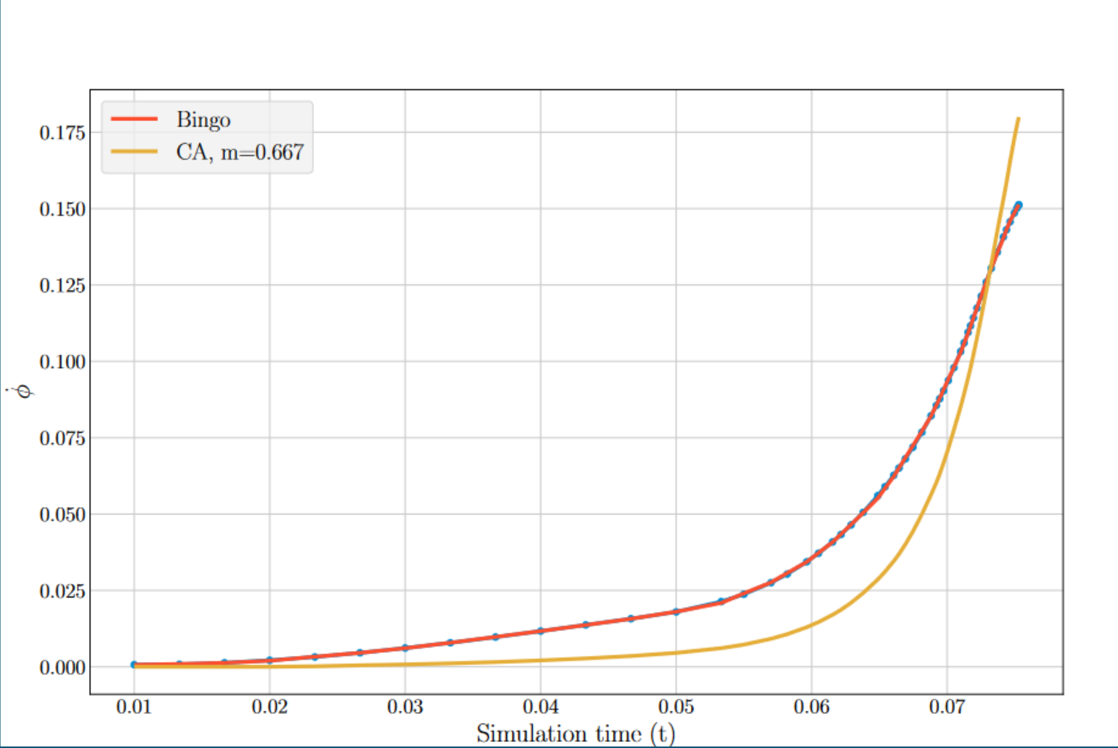
$$\sigma = (1-\phi)\tilde{\sigma}$$

Results and comparison

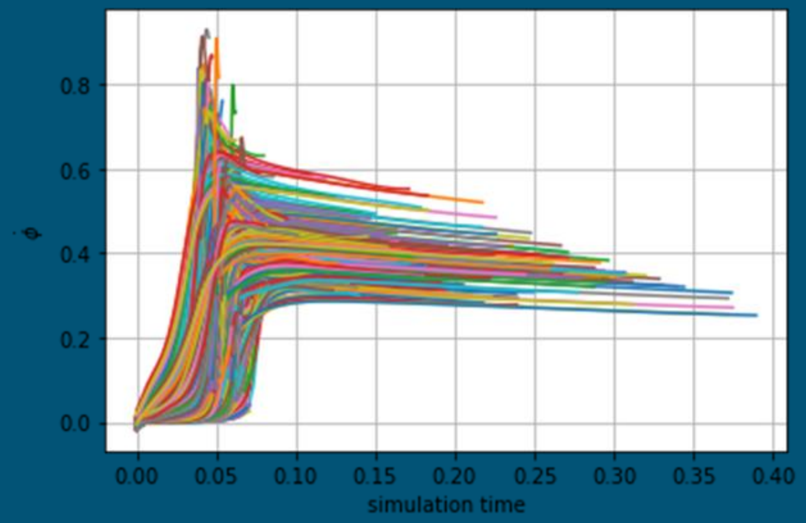
$$\dot{\phi} = \sqrt{\frac{3}{2}}\,\dot{\epsilon}^{p}\,\frac{1-(1-\phi)^{n+1}}{(1-\phi)^{n}}\,\sinh\left[\frac{2(2n-1)}{2n+1}\frac{\sigma_h}{\sigma_e}\right]$$

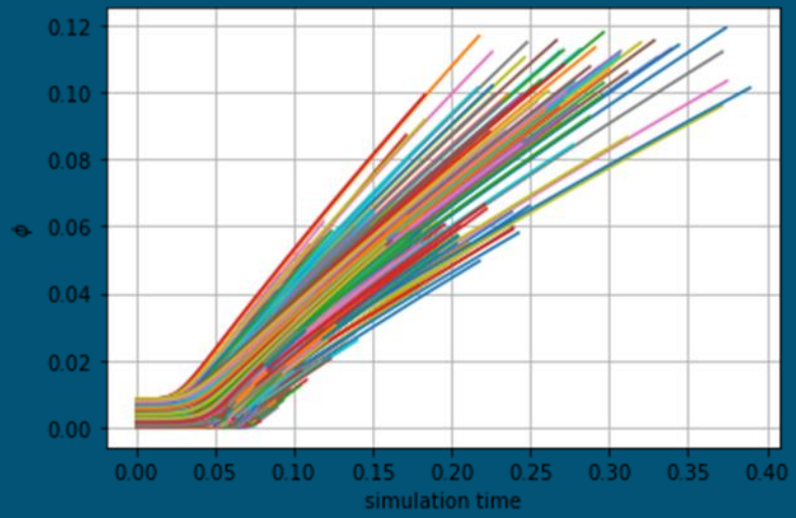
$$\begin{aligned}
&-1266.56465709685\phi T/(\phi - T) + 1.8281231411269e^{-6}T^{2}\cosh(T)\cosh(2T)/(\phi - T)\\
&- 0.000204082955151593T^{2}\cosh(2T)/(\phi - T) - 1.8281231411269e^{-6}T\cosh(T)^{2}\cosh(2T)/(\phi - T)\\
&+ 0.000204082955151593T\cosh(T)\cosh(2T)/(\phi - T) + 0.000743321346813624T\cosh(2T)/(\phi - T)\\
&+ 3000.4565365942T/(\phi - T) + 0.0230704434503944\cosh(T) + 1734.2224438618\\
&- 22299833871536.8/(-104581162220851.0\cosh(2T) - 1.09956329870896e^{15})\\
&- 0.000743321346813624\cosh(T)\cosh(2T)/(\phi - T) - 1733.74640038185/(\phi - T)
\end{aligned}$$

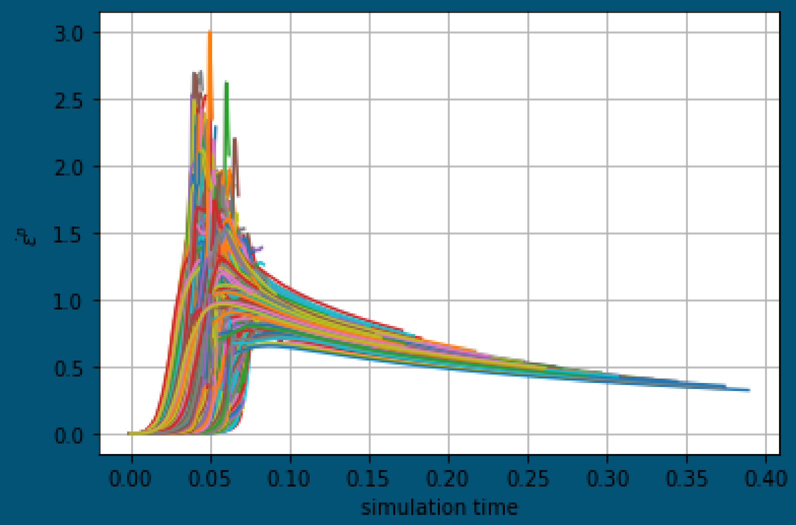


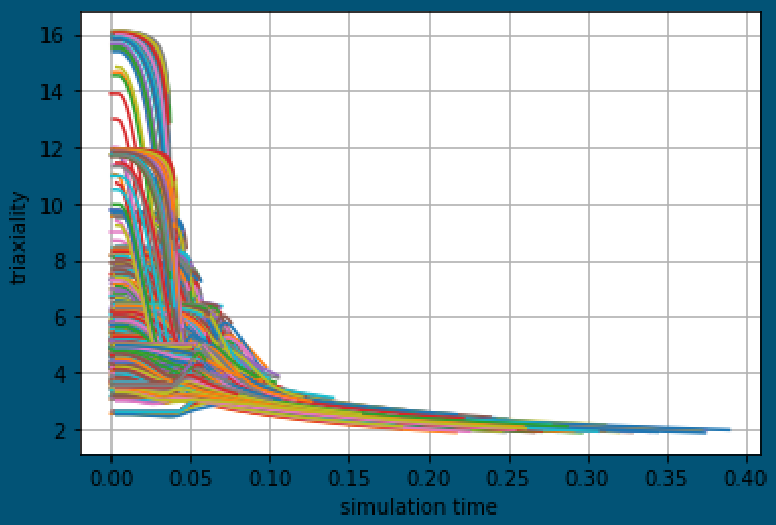


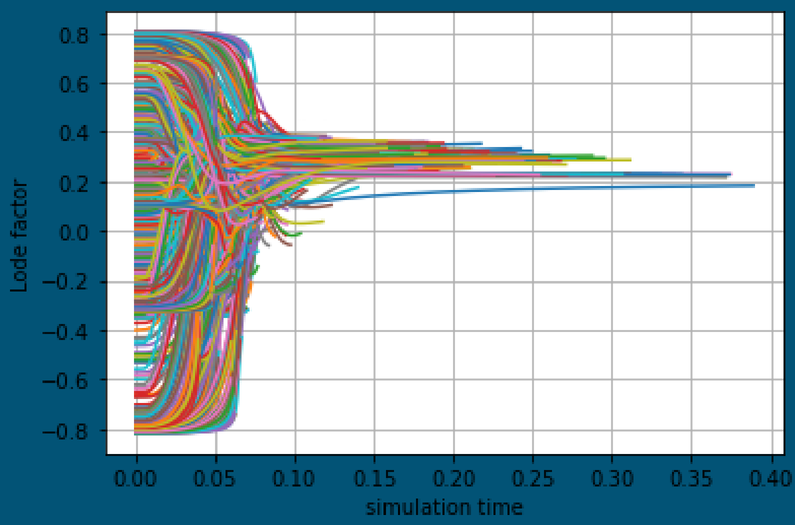
Results and comparison





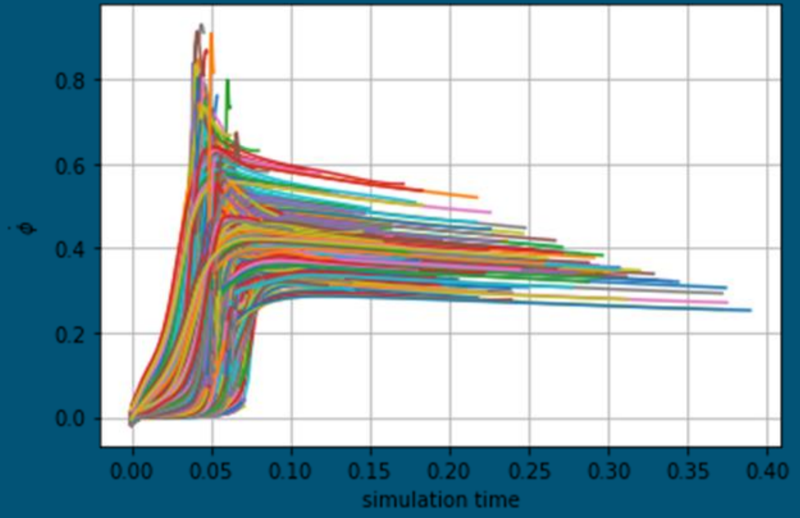




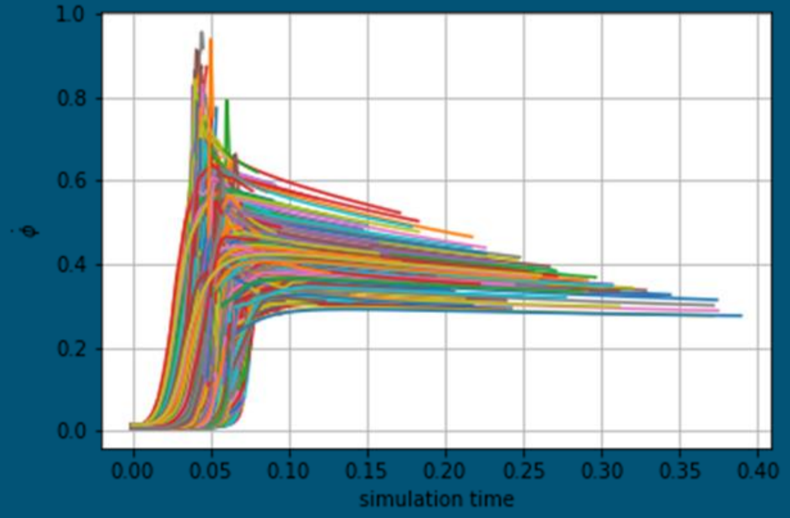


Results and comparison

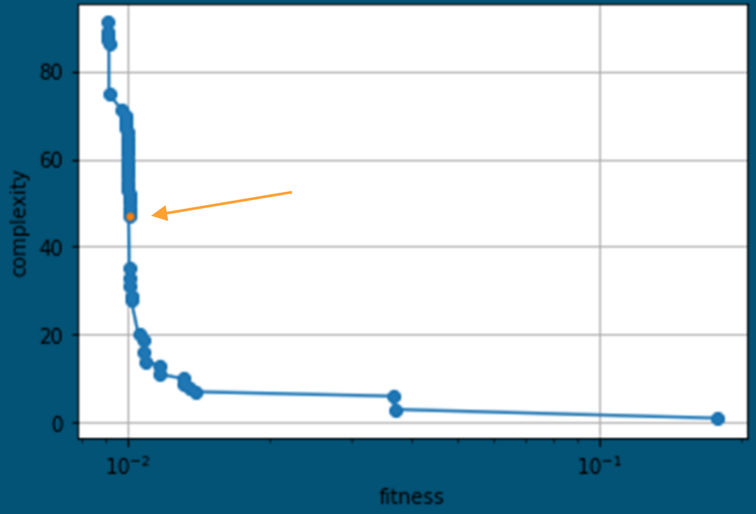
Raw data



Bingo model



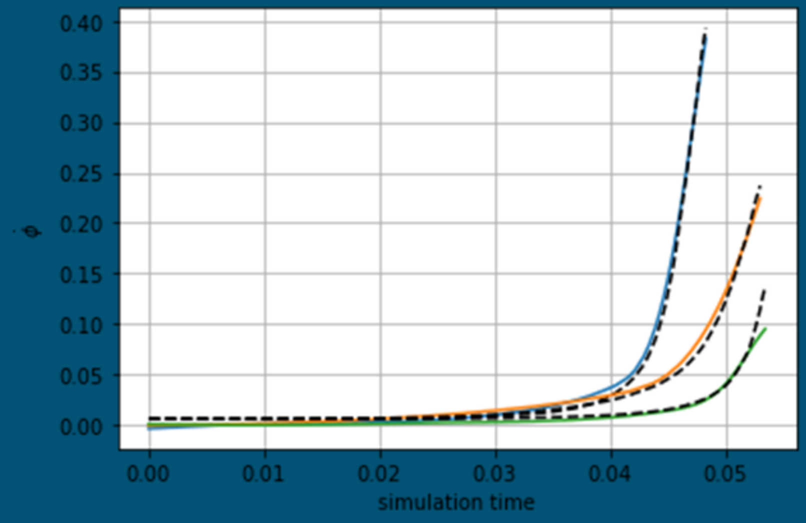
Pareto front

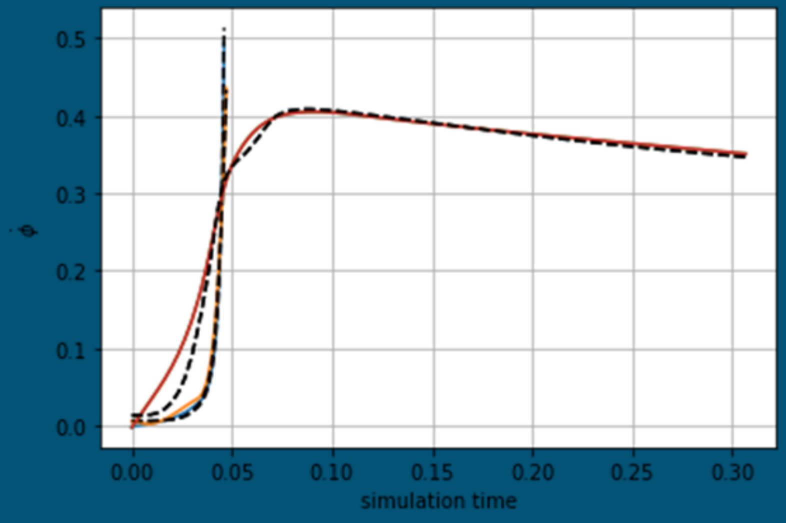


$$\dot{\phi} = \sqrt{\frac{3}{2}}\,\dot{\epsilon}^p\,\frac{1-(1-\phi)^{n+1}}{(1-\phi)^n}\,\sinh\left[\frac{2(2n-1)}{2n+1}\,\frac{\sigma_h}{\sigma_e}\right]$$

$$\begin{gathered}
-0.331601702572\phi^3(\dot{\epsilon}^p)^2T - 2.8e^{-5}\phi^3\dot{\epsilon}^pT + \\
230472.485470718\phi^3\dot{\epsilon}^pT/(-\phi\dot{\epsilon}^p - 115874.234587) + \\
0.32691013712\phi^2(\dot{\epsilon}^p)^2T + 2.8e^{-5}\phi^2\dot{\epsilon}^pT^2 + 2.8e^{-5}\phi^2\dot{\epsilon}^pTL + \\
2.000946907344\phi^2\dot{\epsilon}^pT - 0.331601702572\phi^2\dot{\epsilon}^p - \\
67693.276903898\phi^2\dot{\epsilon}^p/(-\phi\dot{\epsilon}^p - 115874.234587) + \\
2.8e^{-5}\phi^2\sinh(2\dot{\epsilon}^p + 2\cosh(\phi)) - 0.485153643688\phi^2 + 0.491124069968
\end{gathered}$$

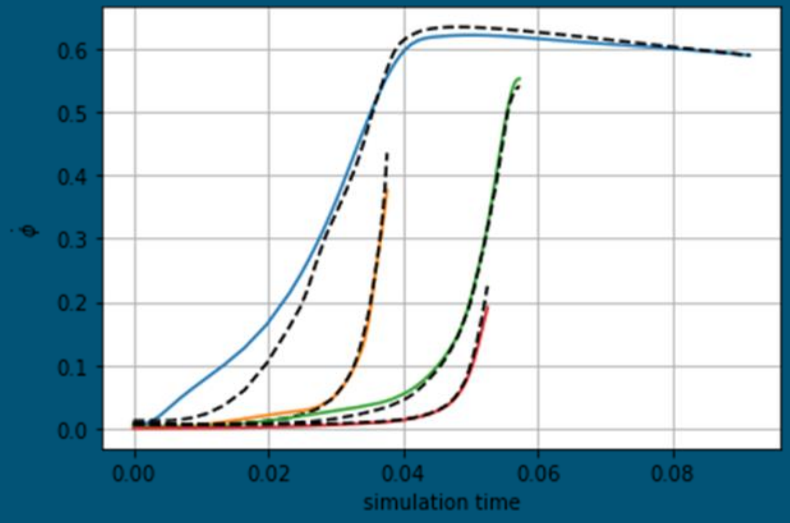
Results and comparison

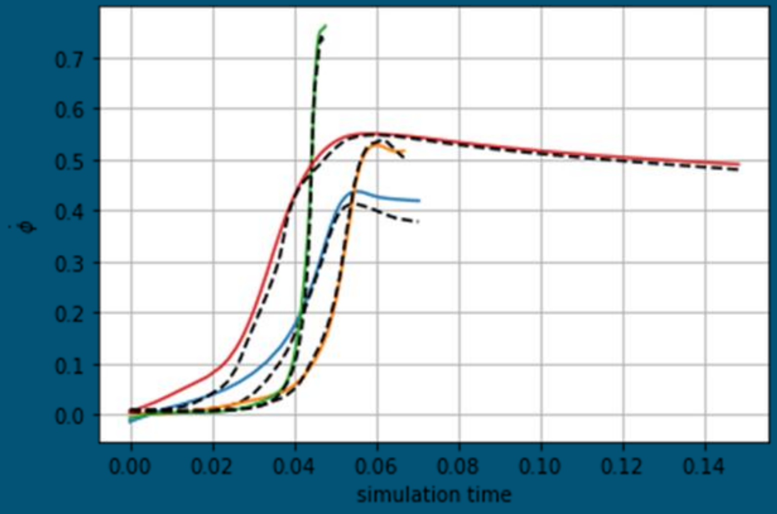


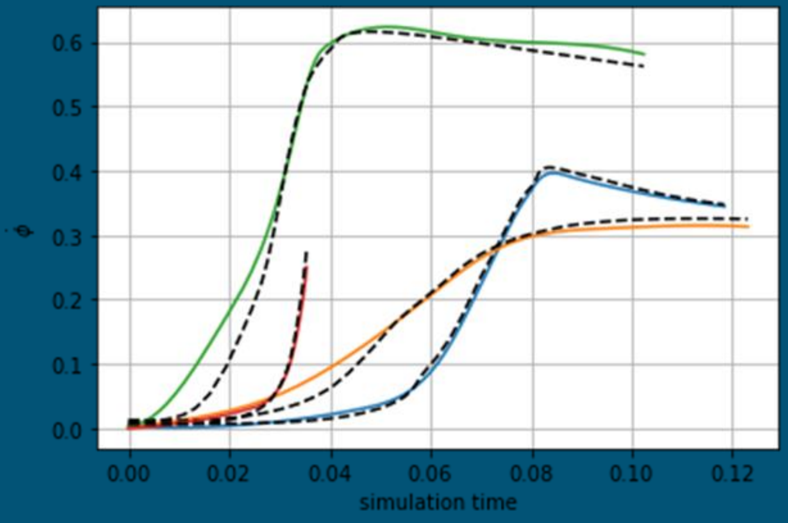


Raw data (solid)

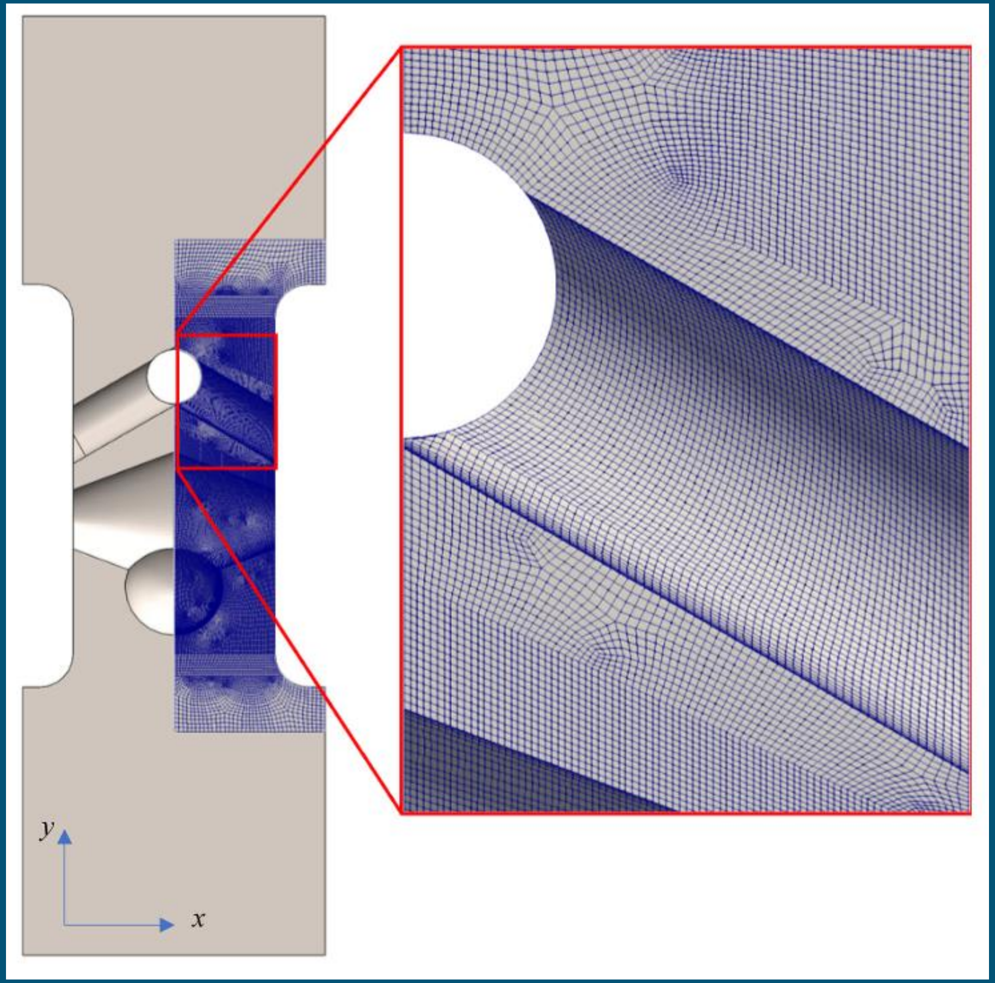
Bingo model (dashed)







Sandia Fracture Challenge



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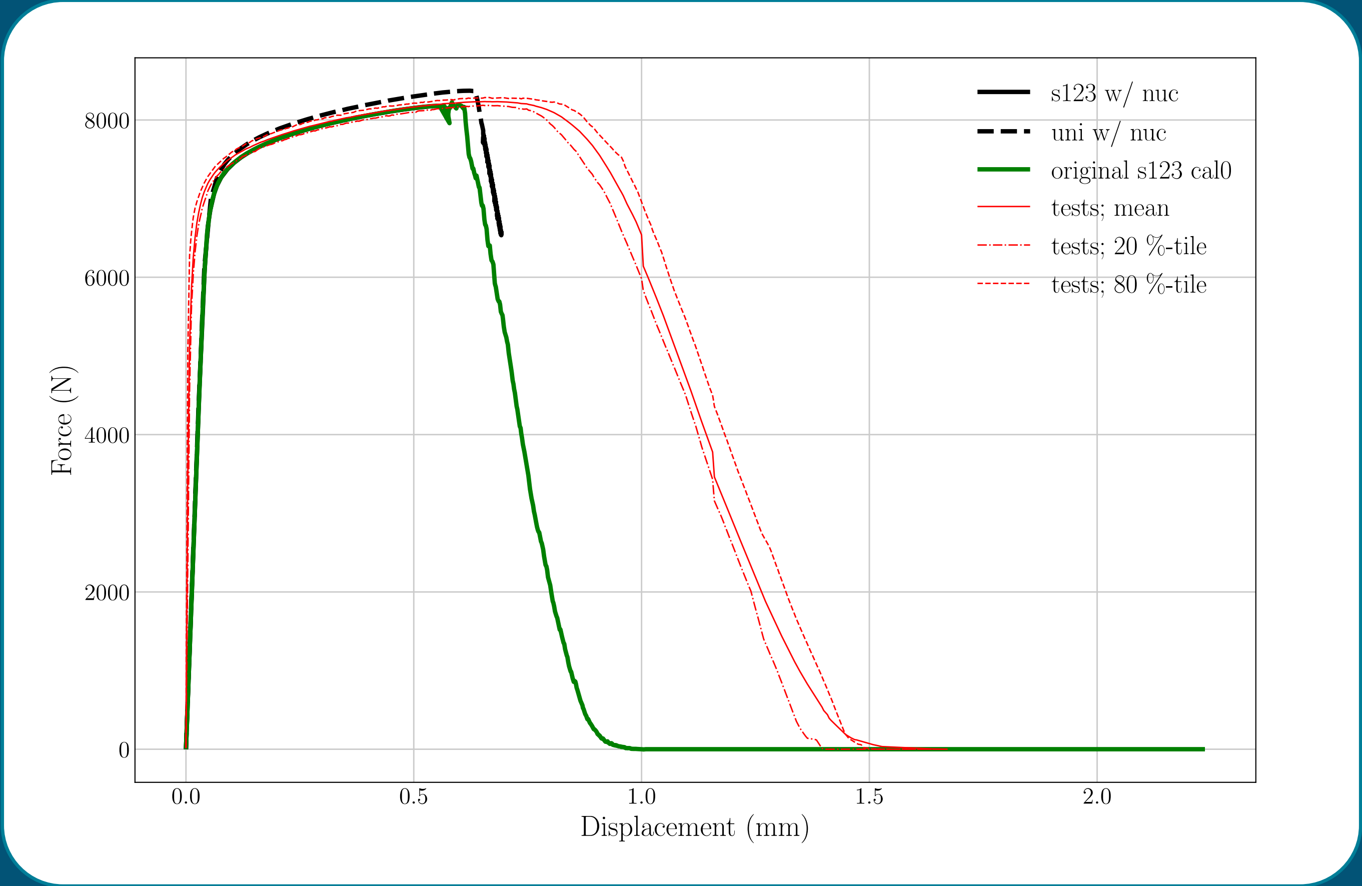
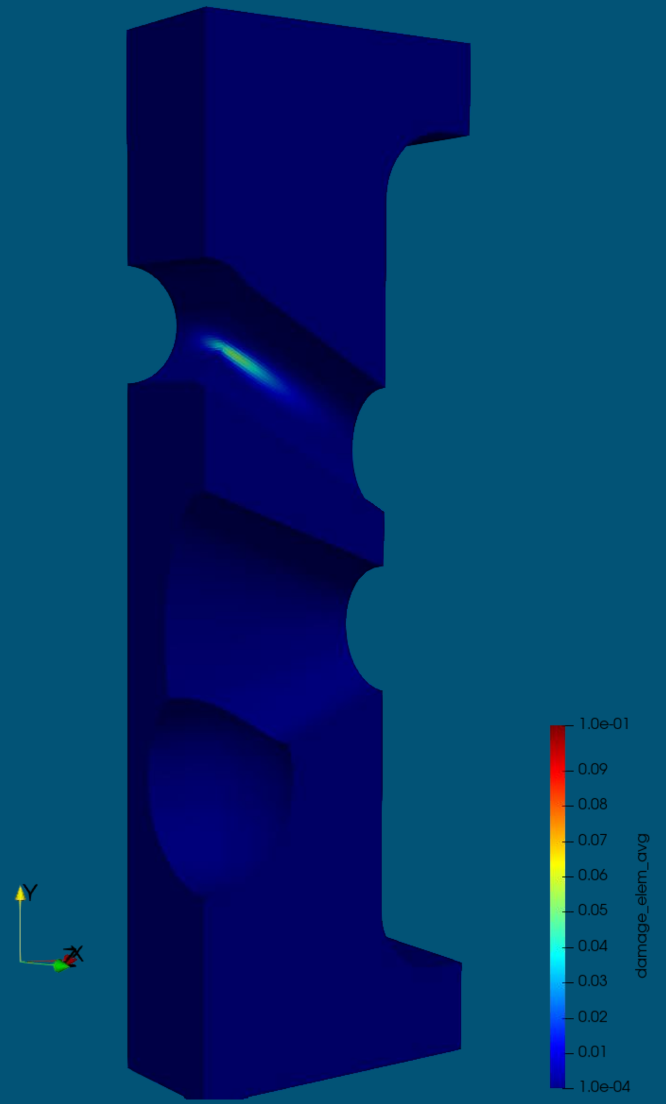
Sandia Fracture Challenge





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[6] Kramer, S.L.B., et al. The third Sandia fracture challenge: predictions of ductile fracture in additively manufactured metal. *Int J. Fract.* **218**, 5-61 (2019).

Conclusion

- GPSR was used to obtain an analytic continuum damage model.
  - Training data for GPSR was provided by DNS.
  - This model was compared with the existing Cocks-Ashby damage model.
  - This model was used to predict fracture of an AM specimen.

- Many considerations going forward:
  - Fitness for (integrated) evolution equations.
  - Model uncertainty quantification[10] or spatially-varying damage models.
  - Refinement of microstructural features.
    - Pore nucleation/coalescence, pore/particle shape, grain morphologies, and related microstructural statistics.
  - Optimized generation of training data.
    - Cognizant of paths through state-variable space, not just applied deformations.
  - Size effects, extreme-value statistics, etc.

[10] Bomarito, G.F., Leser, P.E., Strauss, N.C.M., Garbrecht, K.M., Holchhalter J.D. Automated learning of interpretable models with quantified uncertainty. arXiv:2205.01626 (2022).

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