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Sandia National Laboratories

Developing data-driven strength models incorporating temperature and strain-rate dependencies

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Sandia National Laboratories

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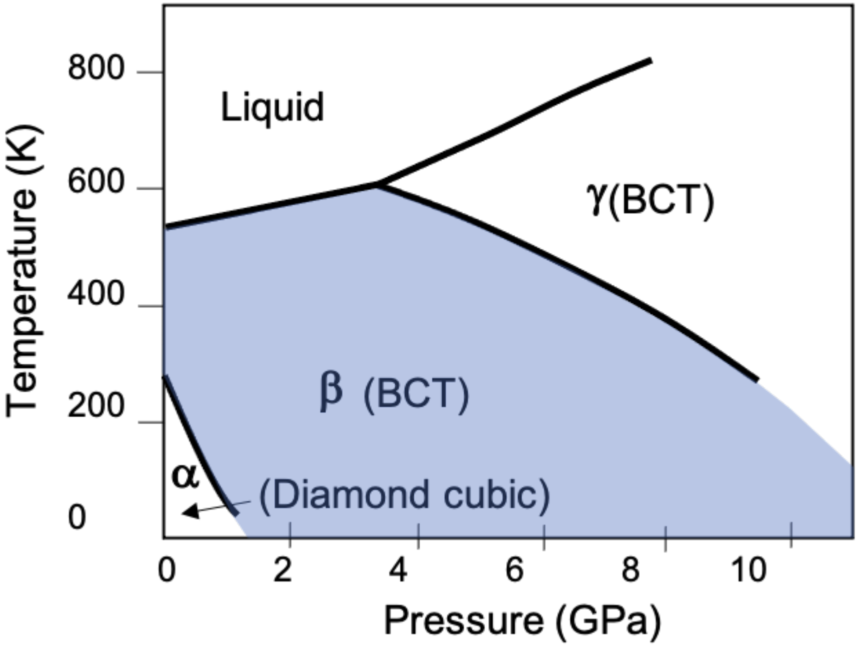
SAND2024-XXXXXC

U.S. DEPARTMENT OF ENERGY

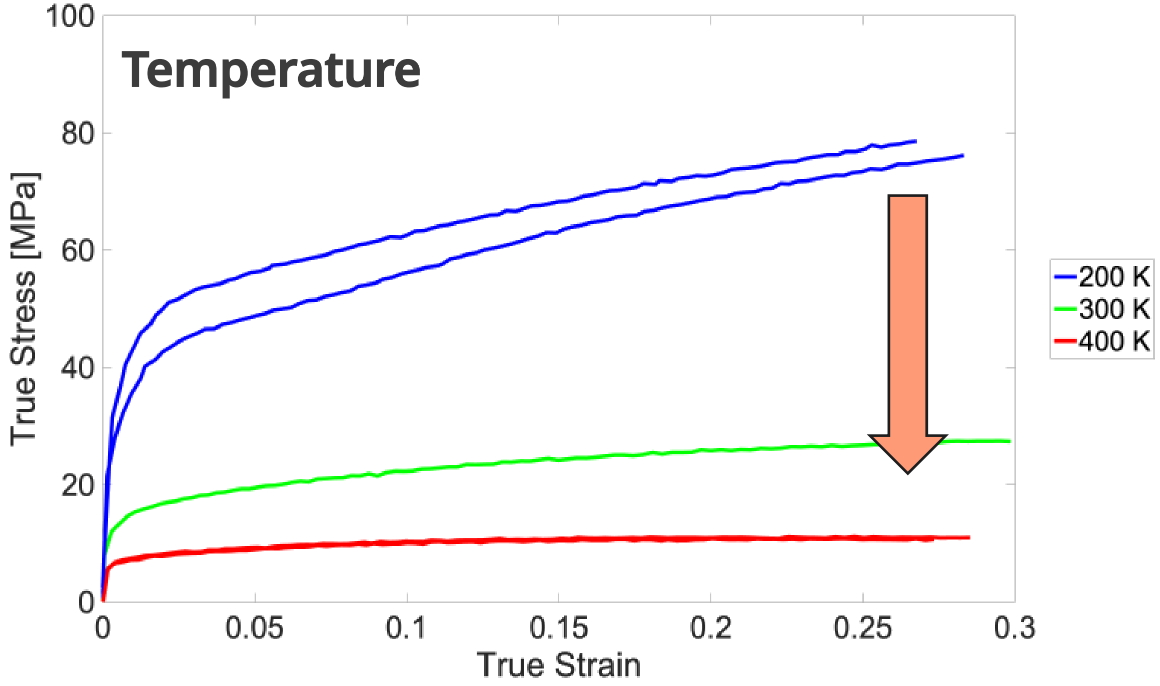
NNSA

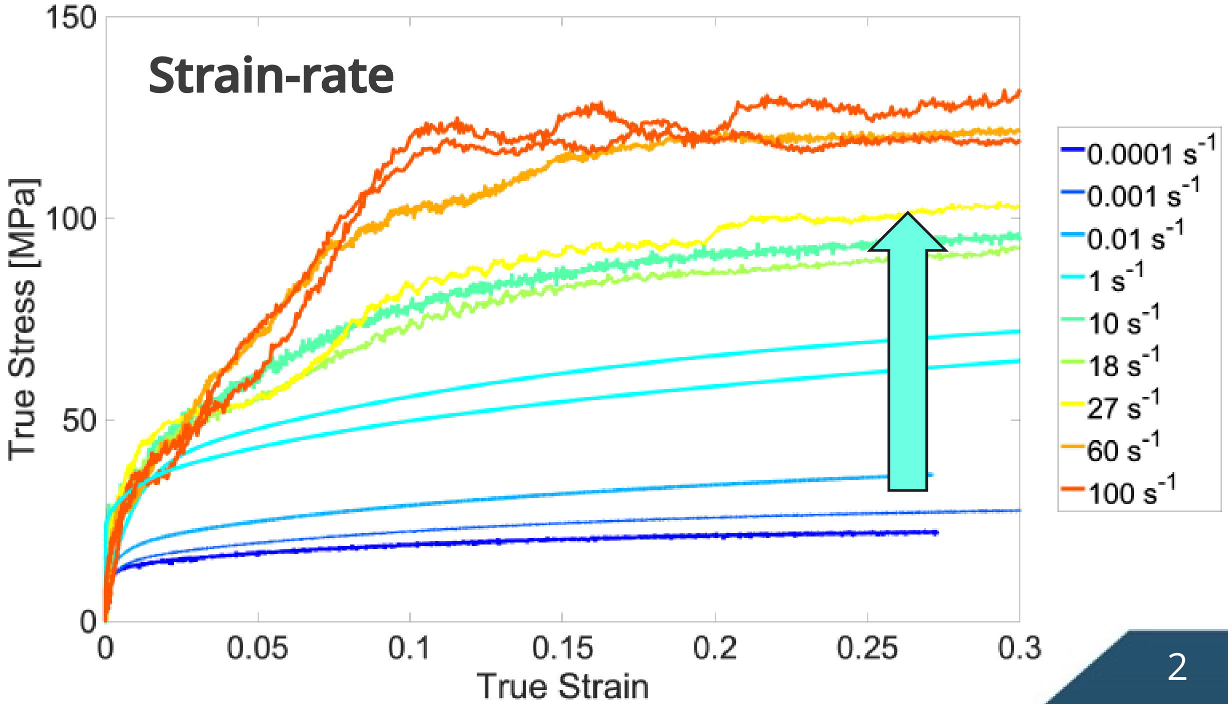
Tin displays complex behavior

- Used in plating, soldering, and alloying
- Low melting temperature (~500 K) and recrystallization temperature (~300 K)
  - Leads to complex microstructural evolution and large distributions in mechanical response



H. Lim et al., SAND Report (2022) - SAND2022-2368

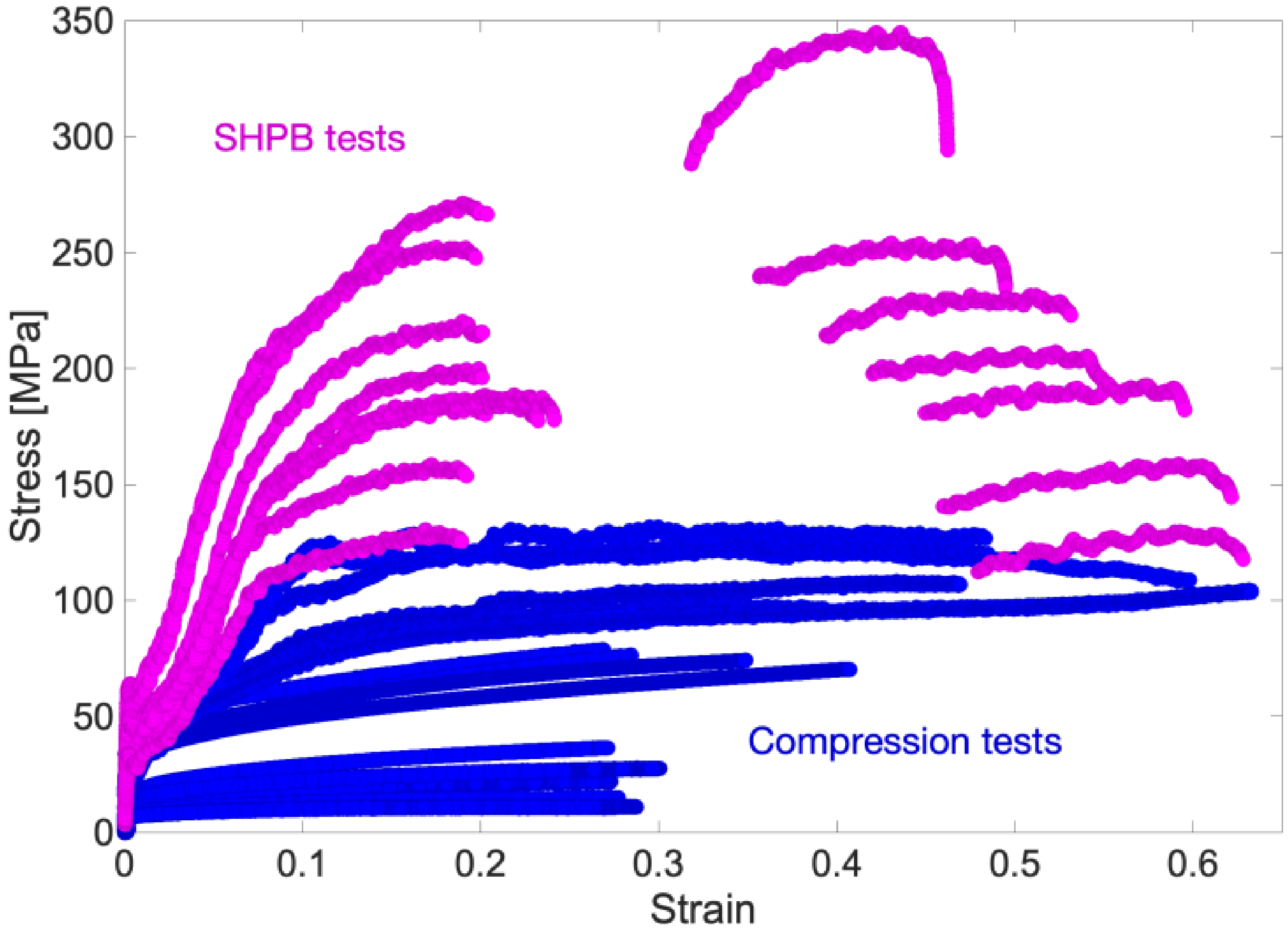




Experimental characterization of β-Tin

- Compression tests
  - Experimentalists: Jay Carroll & Zachary Casias
  - Temperature: $200 \sim 400\ K$
  - Strain-rate: $0.0001 \sim 100\ s^{-1}$

- Split-Hopkinson Pressure Bar (SHPB) tests
  - Experimentalist: Saryu Fensin (Los Alamos)
  - Temperature: $190 \sim 375\ K$
  - Strain-rate: $3175 \sim 3900\ s^{-1}$



H. Lim et al., SAND Report (2022) - SAND2022-2368

Traditional strength models - $\boldsymbol{\sigma = f(\varepsilon, \dot{\varepsilon}, T)}$

Johnson-Cook (JC): **5 parameters**

$$\sigma = (A + B\varepsilon^n)(1 + C ln\dot{\varepsilon})(1 - T^{*m})$$

Zerilli-Armstrong (ZA): **6 parameters**

$$\sigma = C_0 + C_1 \exp(-C_3 T + C_4 T ln\dot{\varepsilon}) + C_5 \varepsilon^{n'}$$

Mechanical Threshold Stress (MTS): **20 parameters**

$$\sigma = \hat{\sigma}_a + \frac{\mu}{\mu_0}[S(\dot{\varepsilon}, T)\hat{\sigma} + S_i(\dot{\varepsilon}, T)\hat{\sigma}_{\mathrm{i}} + S_s(\dot{\varepsilon}, T)\hat{\sigma}_{\mathrm{s}}]$$

Preston-Tonks-Wallace (PTW): **12 parameters**

$$\sigma = 2\mu\left[\hat{\sigma}_s + \frac{1}{p}\left(s_0 - \hat{\sigma}_y\right)\ln\left[1 - \left(1 - \exp\left(-p\frac{\hat{\sigma}_s - \hat{\sigma}_y}{s_0 - \hat{\sigma}_y}\right)\right)\exp\left(-\frac{p\theta\psi}{\left(s_0 - \hat{\sigma}_y\right)\left[\exp\left[p\left(\frac{\hat{\sigma}_s - \hat{\sigma}_y}{s_0 - \hat{\sigma}_y}\right)\right] - 1\right]}\right)\right]\right]$$

Limitations

- Fixed form
- Extrapolation is difficult
- Multiple parameters to fit
- Assumption-based

Can genetic programming be an alternative method?

Input

Experimental Stress-strain curves

Feature Engineering

$$\varepsilon^* = \varepsilon^{0.396}$$
$$\dot{\varepsilon}^* = \ln(\dot{\varepsilon})$$
$$T^* = \frac{T}{505\ K}$$

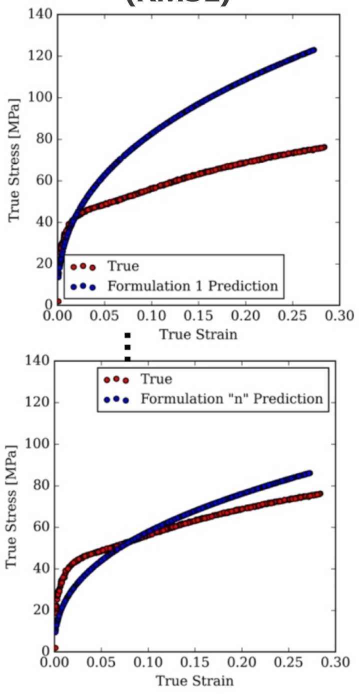
Hyperparameters

Monte Carlo sampling

Population size
Tournament size
Parsimony coefficient

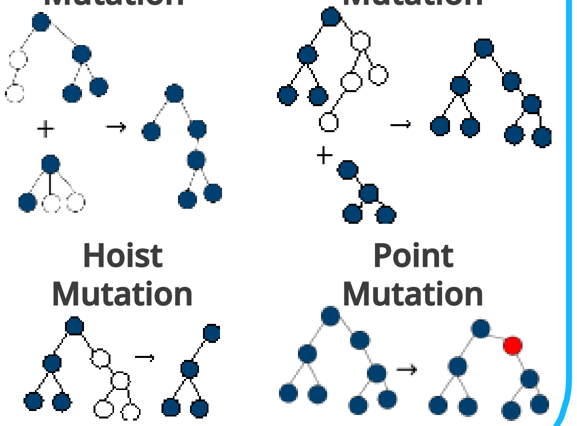
Initial set of naive random formulations
$+, -, \div, \times, \exp(), \sqrt{}$

Evaluate fitness of formulations
(RMSE)



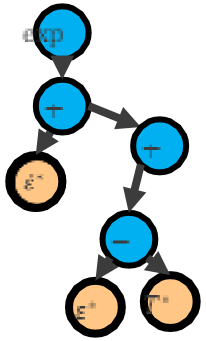
Select top *K* formulations
(Tournament Selection)

Generate new set of formulations by performing genetic operations on fittest formulations



Output

Best Model (example)

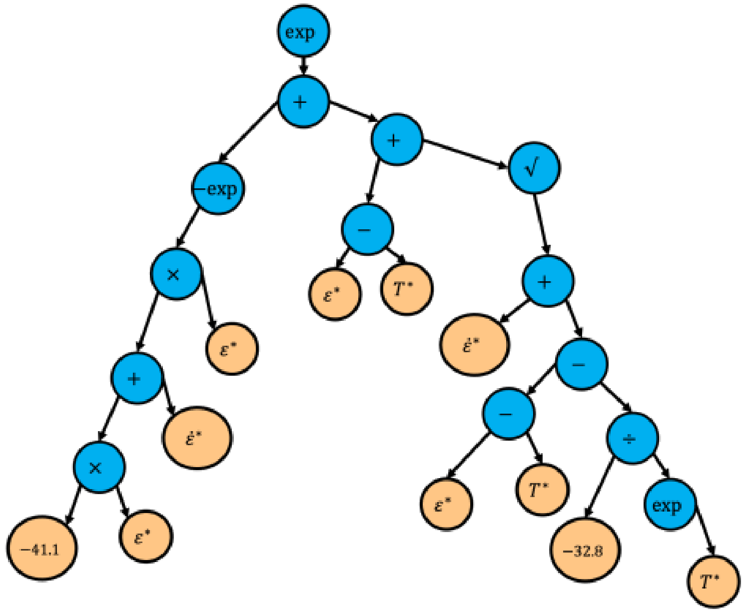


Best model had:

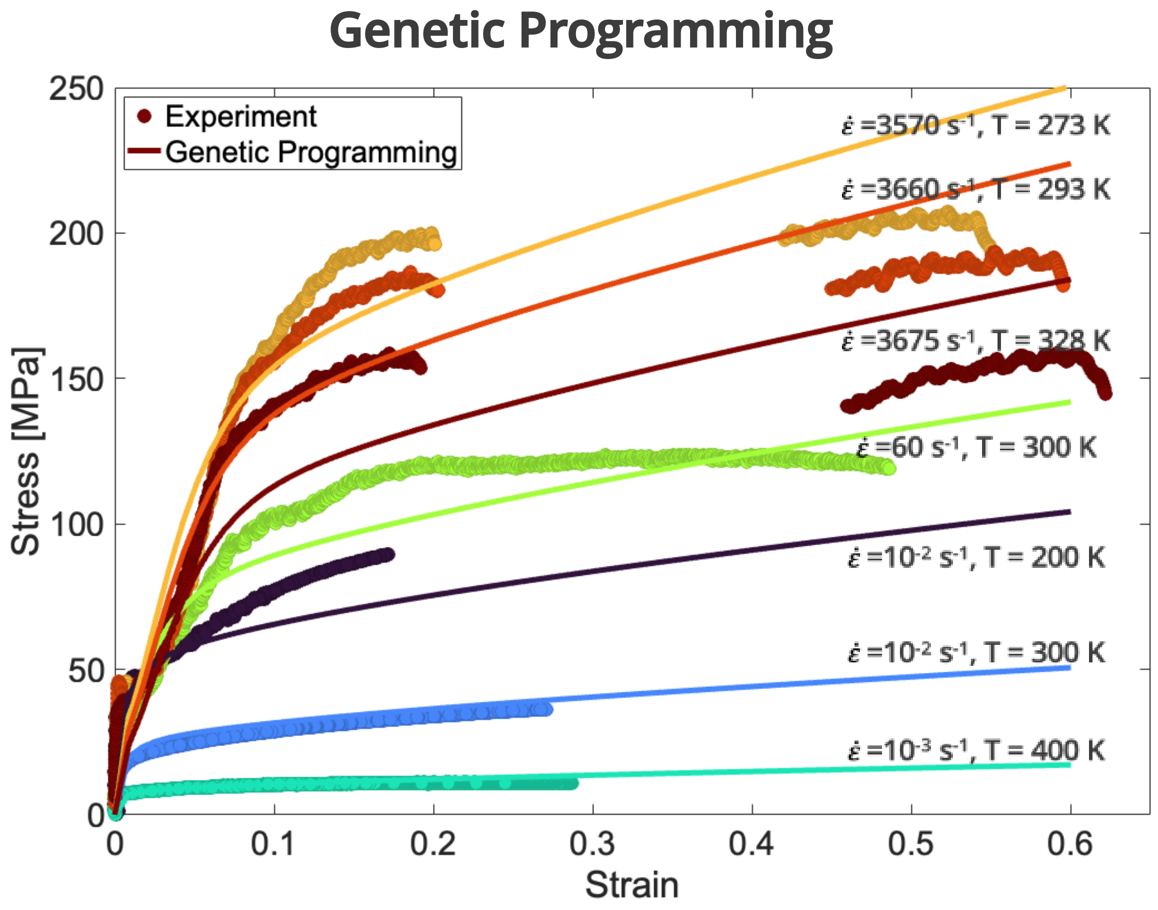
- Lowest RMSE
- Smallest change in RMSE between the training and test sets

D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

What did genetic programming predict to be the best model?



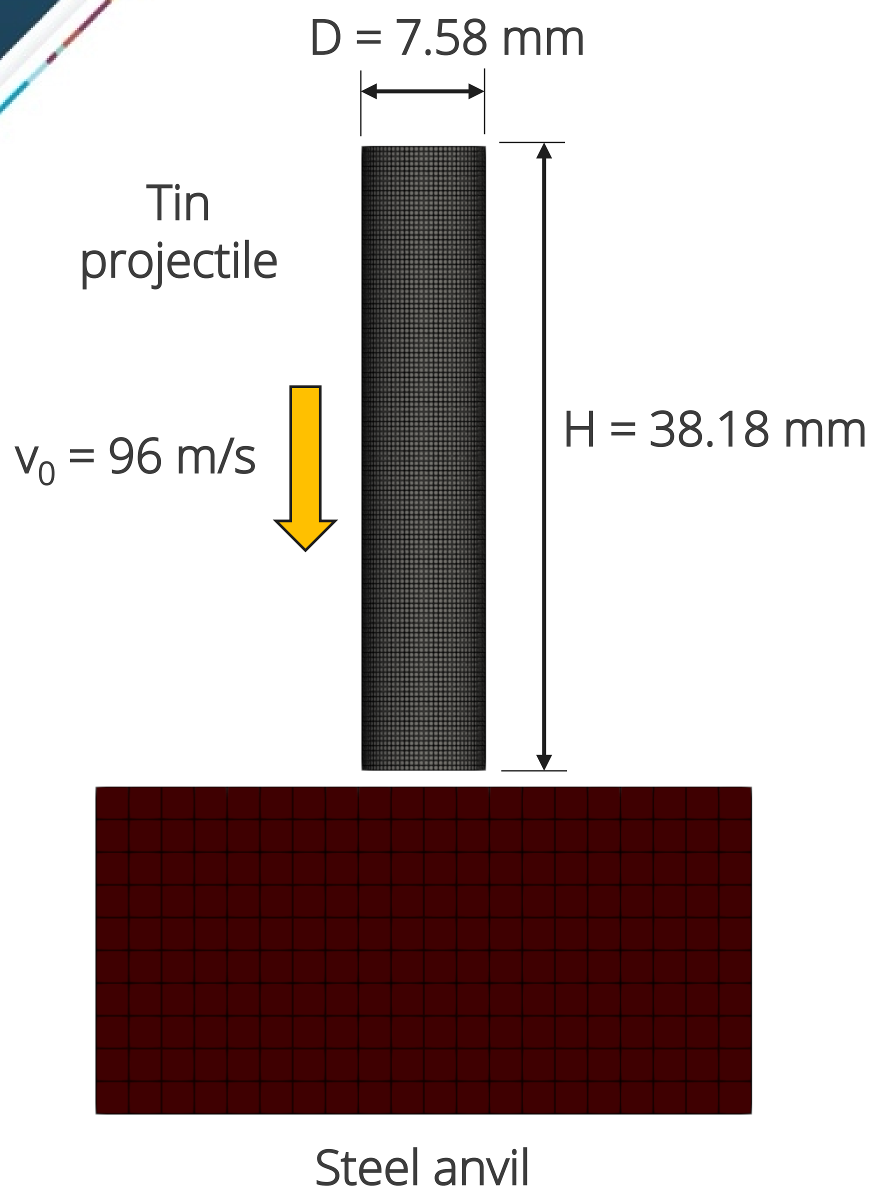
$$\sigma = e^{\left(\left(-e^{\left((C_1\varepsilon^* + \dot{\varepsilon}^*)\varepsilon^*\right)}\right) + \left((\varepsilon^* - X_2) + \sqrt{\dot{\varepsilon}^* + \left((\varepsilon^* - T^*) - \left(\frac{C_2}{e^{T^*}}\right)\right)}\right)\right)}$$



RMSE ~ 14 MPa

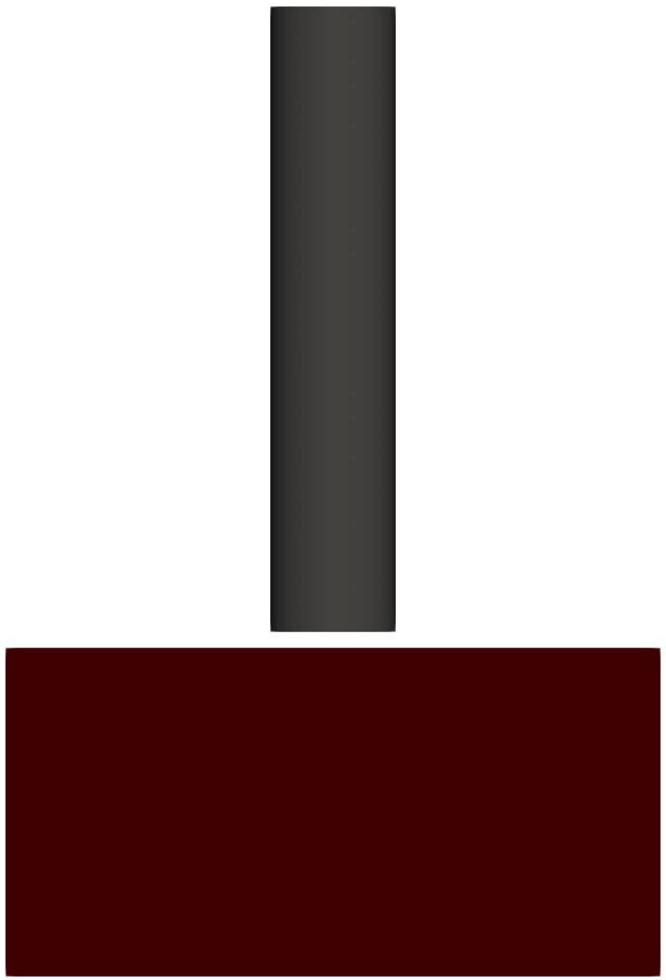
D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

Testing the GP model with the Taylor impact test

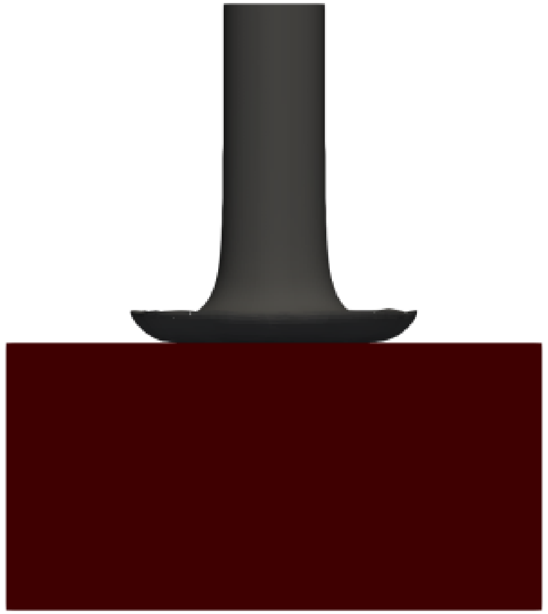


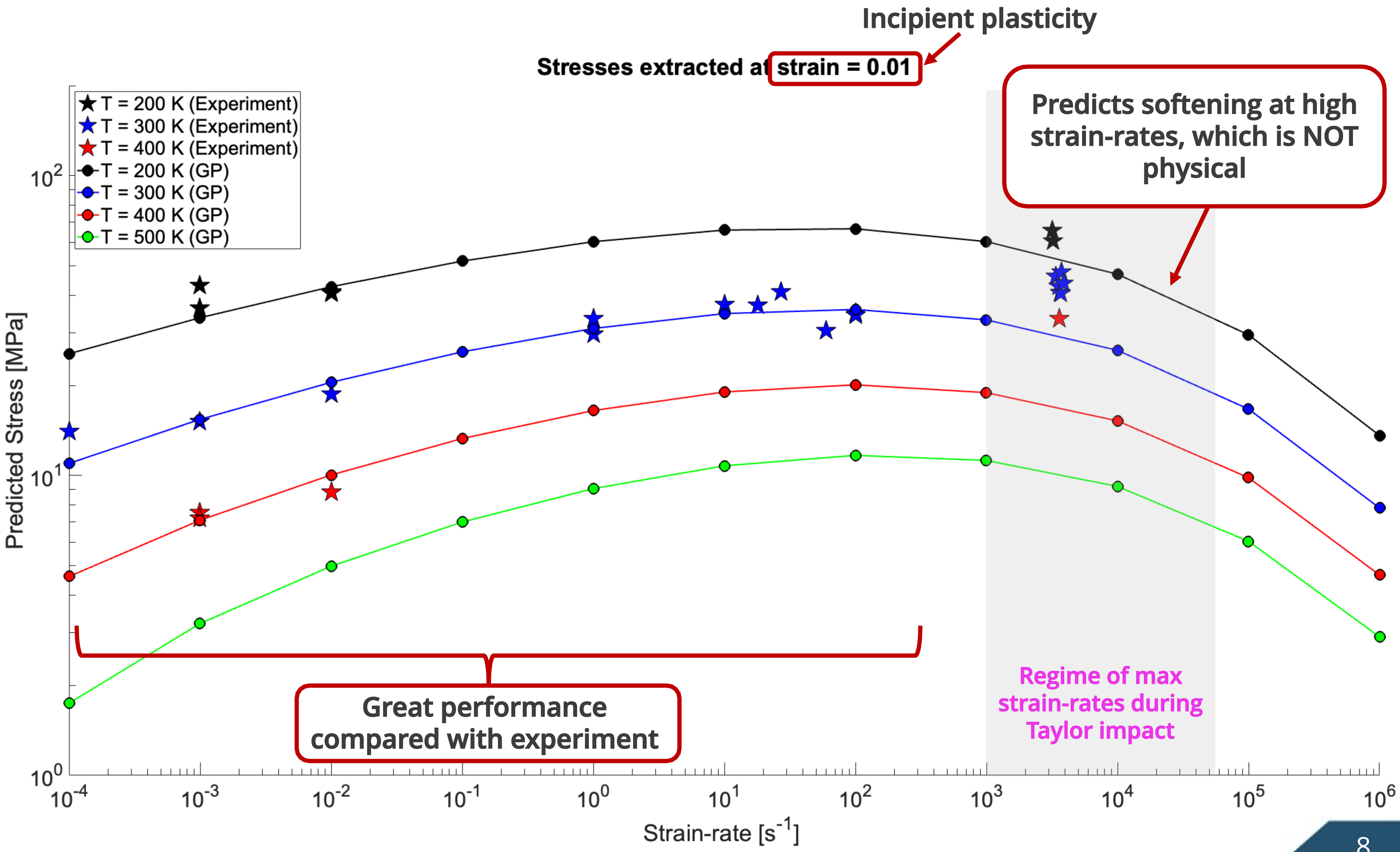
- Simple technique to study dynamic behaviors
  - Strain-rates: $10^{-4} \sim 10^{4}\ s^{-1}$
- Implemented within Sandia's multiphysics shock-hydrodynamics code (*ALEGRA*)
- Material definition:
  - Equation of State: Sesame 2101
  - Yield Model:
    - Johnson-Cook
    - Zerilli-Armstrong
    - Preston-Tonks-Wallace
    - Genetic Programming

Genetic Programming



Why such a soft response from the GP model?





J.R. Koza, Statistics and Computing (1994)
Y. Wang et al., MRS Comm. (2019)

Improving on GP model development

Input

Experimental Stress-strain curves

Feature Engineering

$$\varepsilon^* = \varepsilon$$
$$\dot{\varepsilon}^* = \ln(\dot{\varepsilon})$$
$$T^* = \frac{T}{505\ K}$$

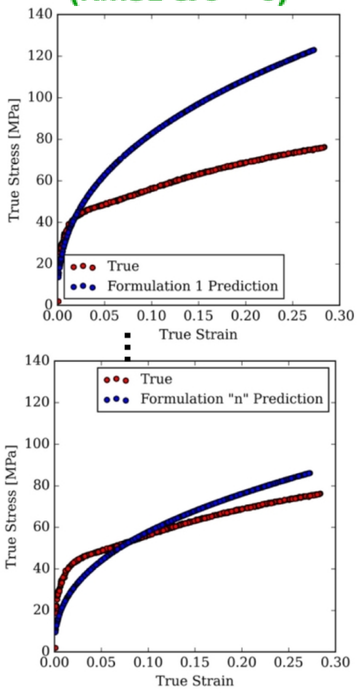
Hyperparameters

Bayesian optimization

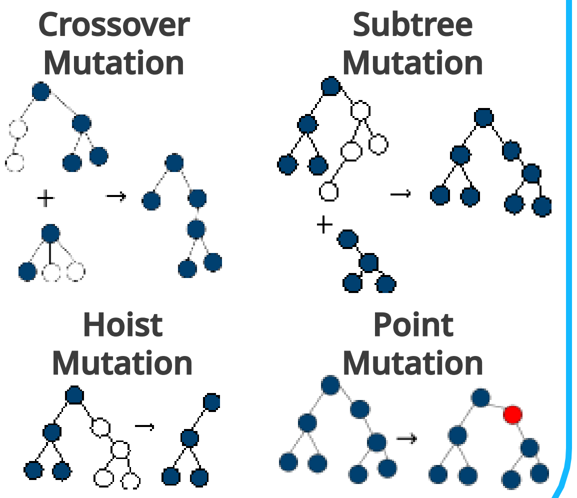
Population size
Tournament size
Parsimony coefficient

Initial set of naive random formulations
$+, -, \div, \times, \exp(), \sqrt{}$

Evaluate fitness of formulations
(RMSE & $\sigma > 0$)



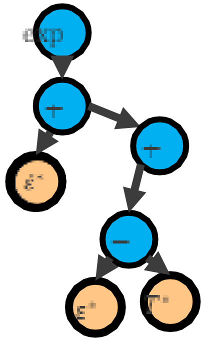
Generate new set of formulations by performing genetic operations on fittest formulations



Select top *K* formulations
(Tournament Selection)

Output

Best Model (example)

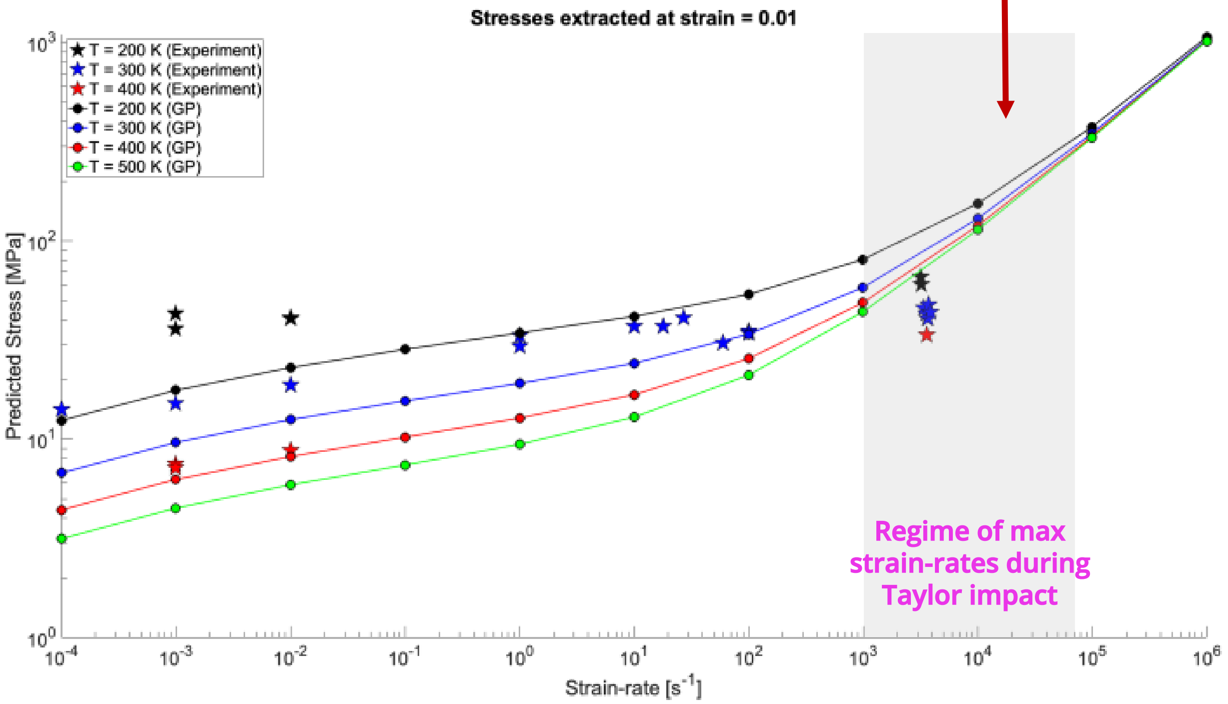


Best model had:

- Lowest RMSE
- $\frac{\partial \sigma}{\partial \dot{\varepsilon}} \geq 0$
- $\frac{\partial \sigma}{\partial \varepsilon} \geq 0$

New and improved GP model

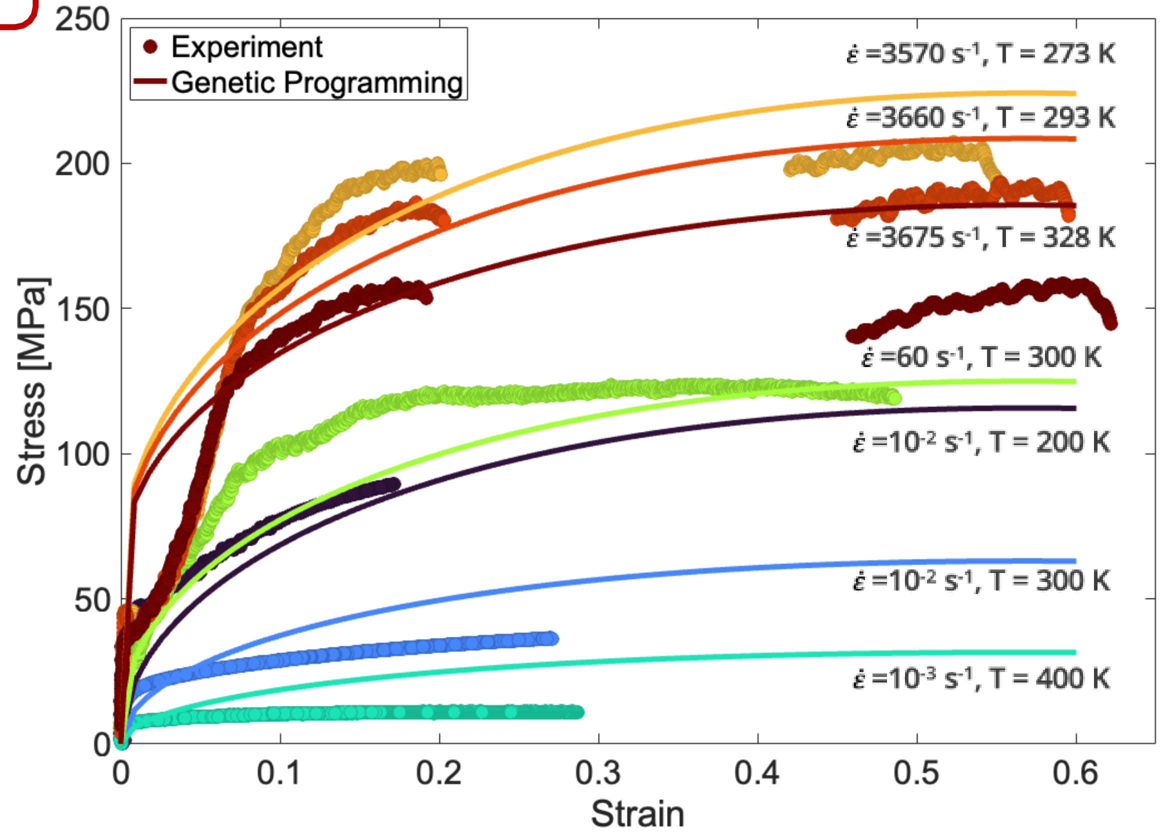
Does not predict softening at high strain-rates



Regime of max strain-rates during Taylor impact

$$\sigma = \sqrt{e^{\dot{\varepsilon}^*}} - \frac{(C_1 - 3\dot{\varepsilon}^*)(C_4 - C_3\varepsilon)}{C_2 T^* \sqrt{\frac{T^*}{\varepsilon}}}$$

Genetic Programming

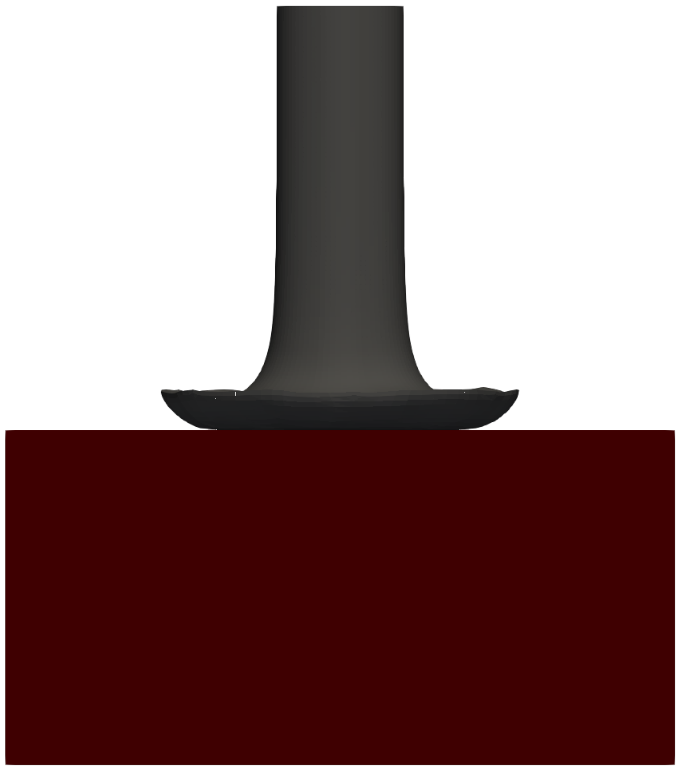


RMSE ~ 20 MPa

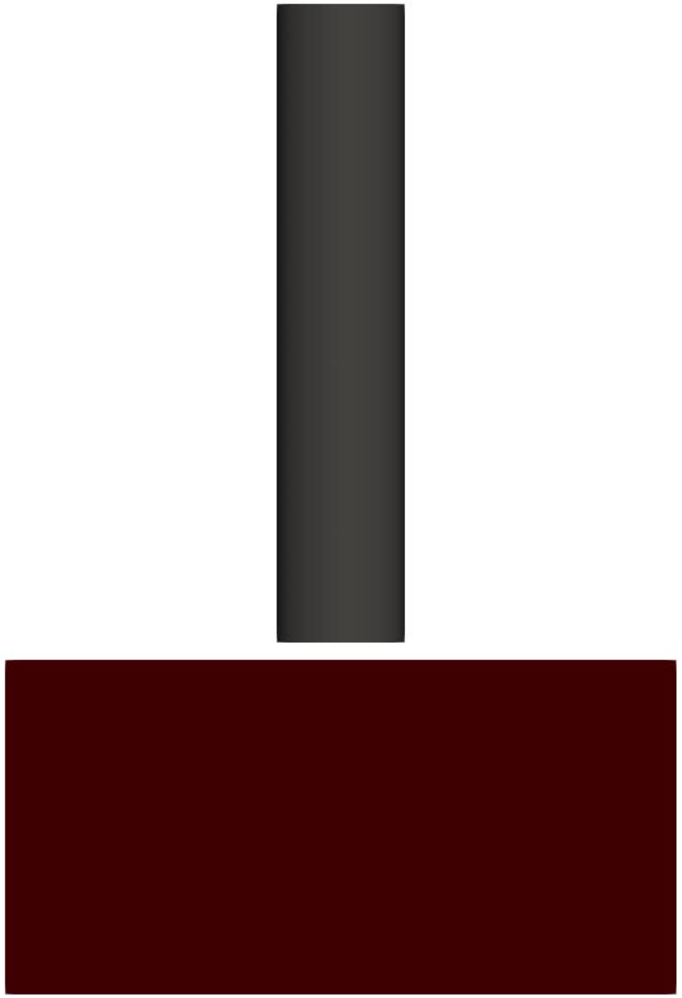
Increase in RMSE

Comparison with previous GP model

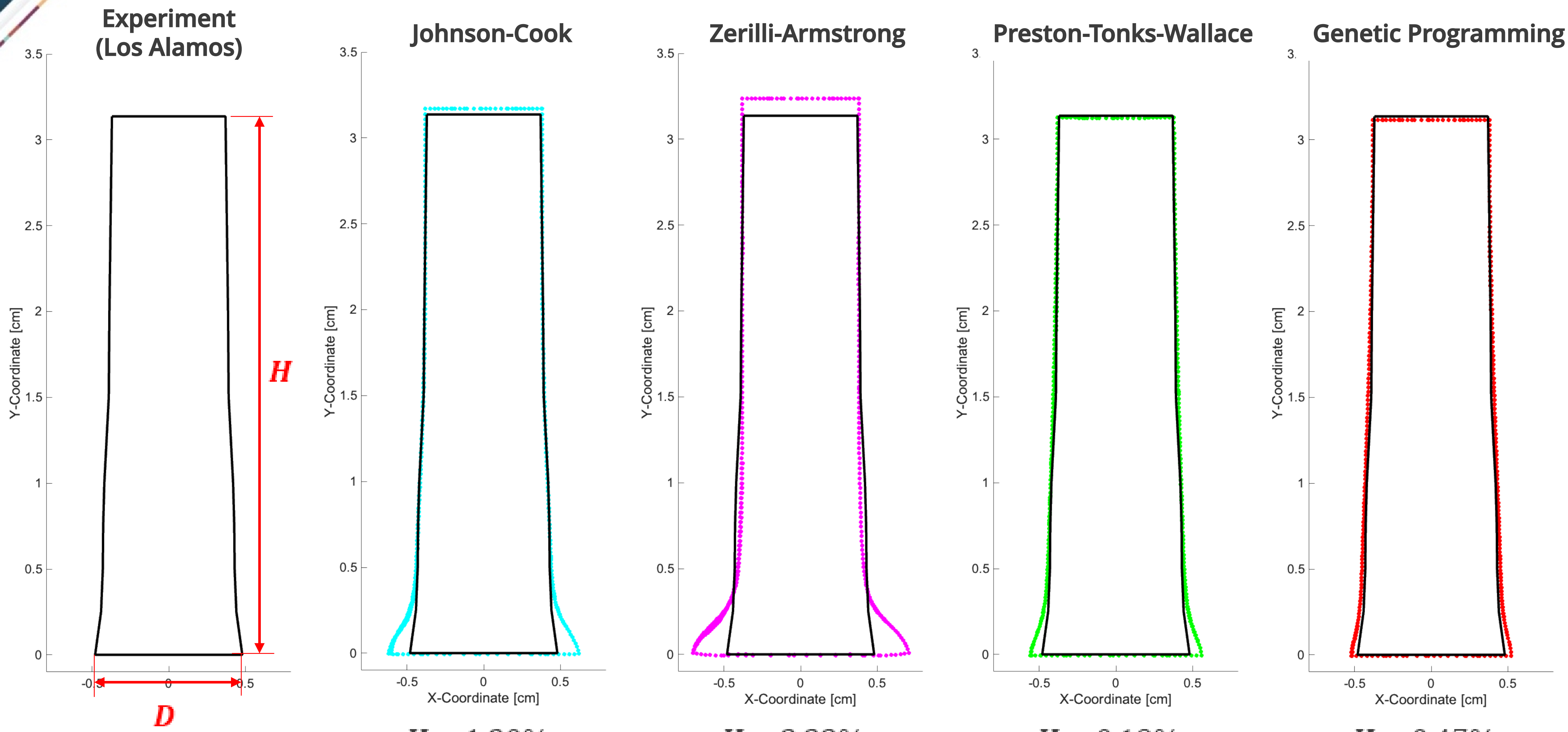
Previous GP model



New GP model



Comparison with traditional models and experiment



Percent Error:

Johnson-Cook: $H \sim 1.20\%$, $D \sim 28.95\%$

Zerilli-Armstrong: $H \sim 3.33\%$, $D \sim 46.78\%$

Preston-Tonks-Wallace: $H \sim 0.19\%$, $D \sim 16.10\%$

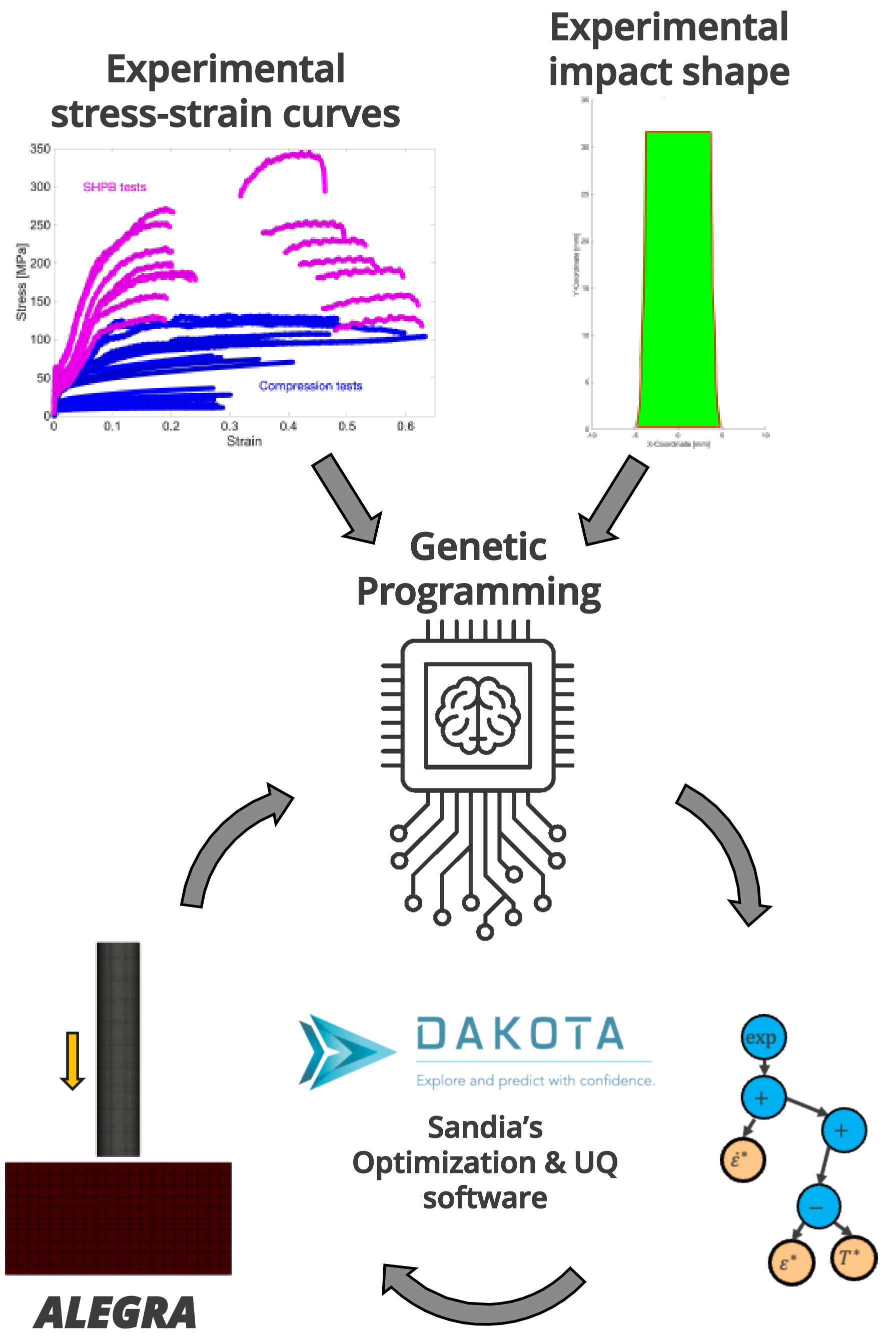
Genetic Programming: $H \sim 0.47\%$, $D \sim 8.88\%$

Conclusions

- Genetic programming (GP) is a novel, useful, and easy way to generate strength models for complex materials at a wide range of temperatures and strain-rates

- Along with experimental data, GP models need physical constraints to predict realistic material behavior

- Future work:
  - Introduce new inputs to GP model from experimental Taylor impact tests (radii, heights)
    - Create a feedback loop that optimizes formulated models by evaluating their hydrocode simulation results



Thank You!

Supplementary

J.R. Koza, Statistics and Computing (1994)
Y. Wang et al., MRS Comm. (2019)

Can genetic programming be an alternative method?

Input

Experimental Stress-strain curves

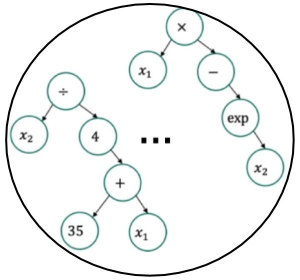
Feature Engineering

$$\dot{\varepsilon}^* = \ln(\dot{\varepsilon})$$

$$\varepsilon^* = \varepsilon^{0.396}$$

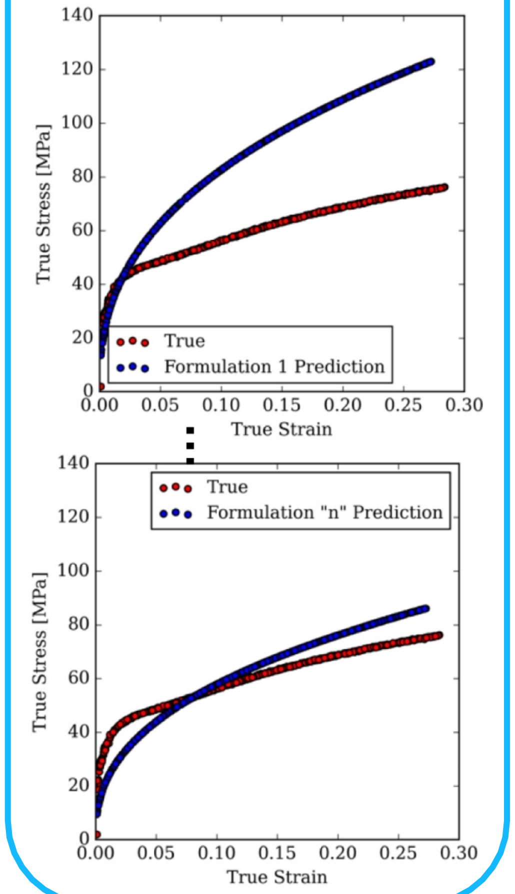
$$T^* = \frac{T}{505\ K}$$

Initial set of random formulations



Arithmetic Operations Explored: $+, -, \div, \times, \exp(), \sqrt{}$

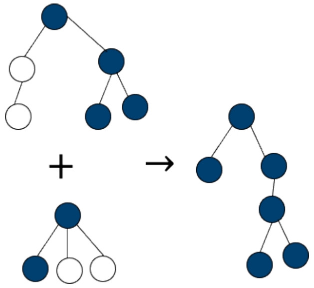
Evaluate fitness of formulations (RMSE)



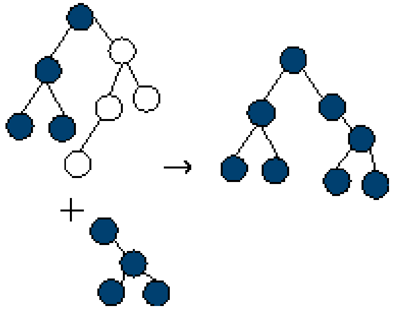
Select top *K* formulations (Tournament Selection)

Generate new set of formulations by performing genetic operations on fittest formulations

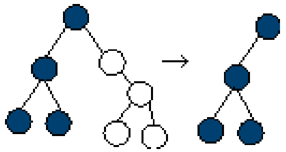
Crossover Mutation



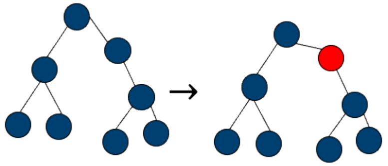
Subtree Mutation



Hoist Mutation



Point Mutation



Continues for *N* generations

D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

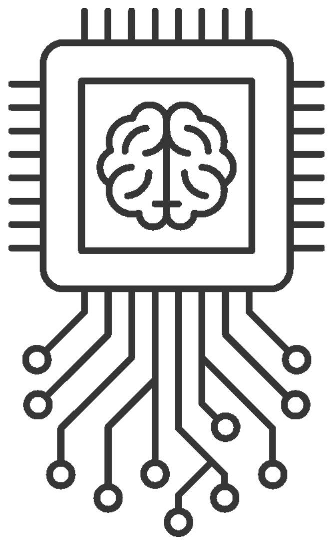
Selecting hyper-parameters using Monte Carlo sampling

Population size
Number of formulations generated

Tournament size
Randomly samples subsets of population

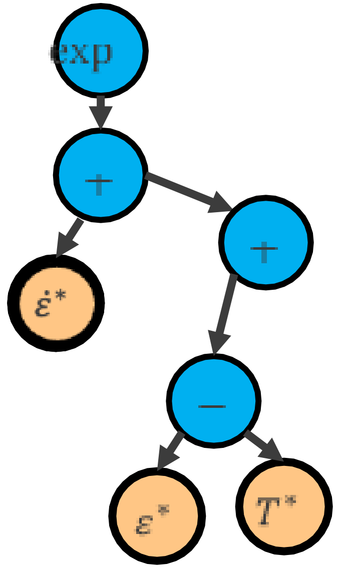
Parsimony coefficient
Penalty to overly complex formulations

Genetic Programming



Continues for *40* generations

Best Model
(example)

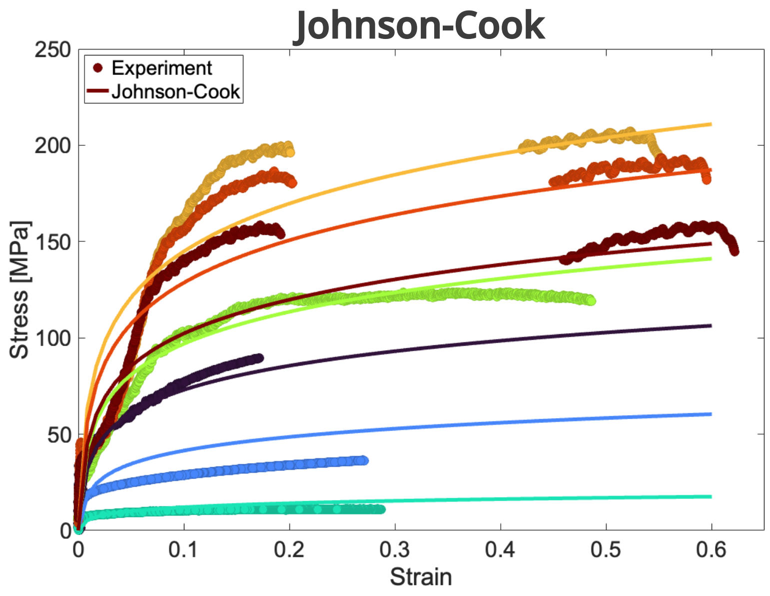


Monte Carlo Sampling (200 samples)

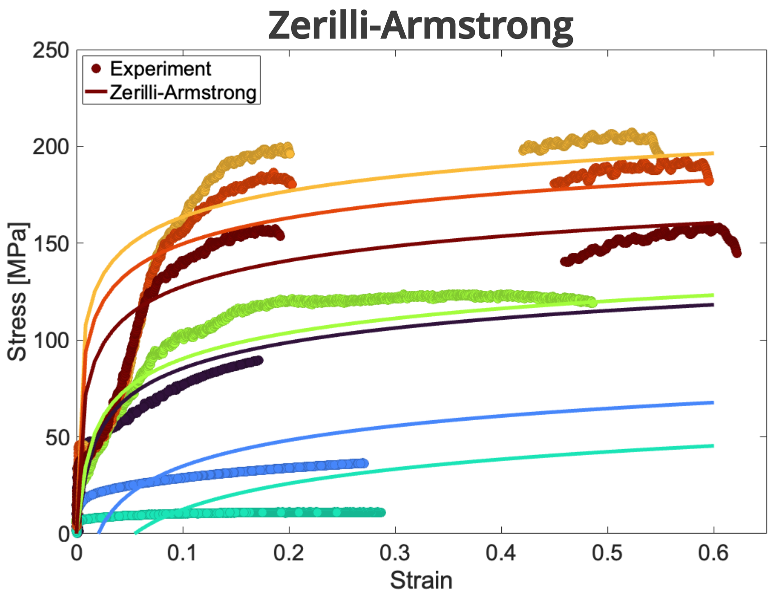
Population	50~50000
Tournament Size	10~1000
Parsimony Coefficient	0.001~0.01

- Best model chosen from hyper-parameters that yielded the lowest RMSE value and had the smallest difference in performance between the training and test sets

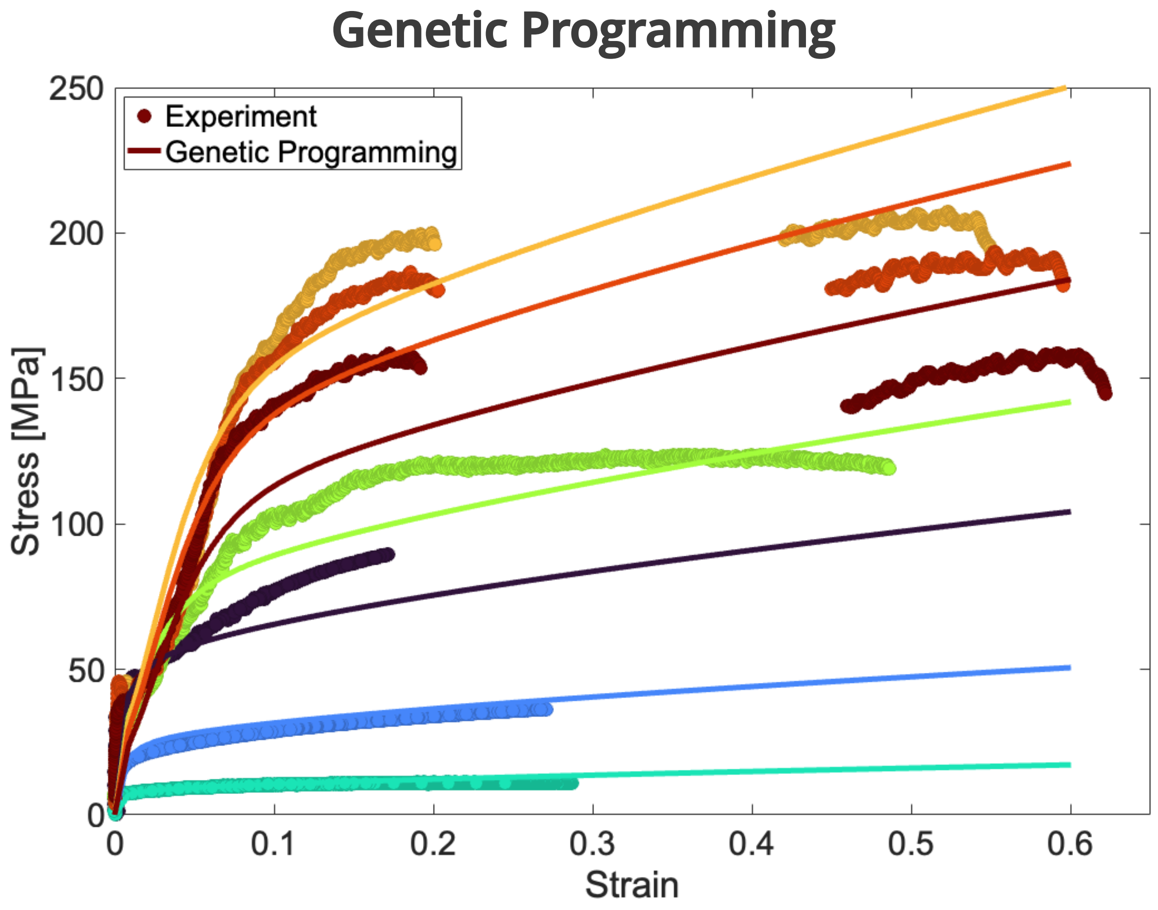
Comparison with traditional models



RMSE ~19 MPa



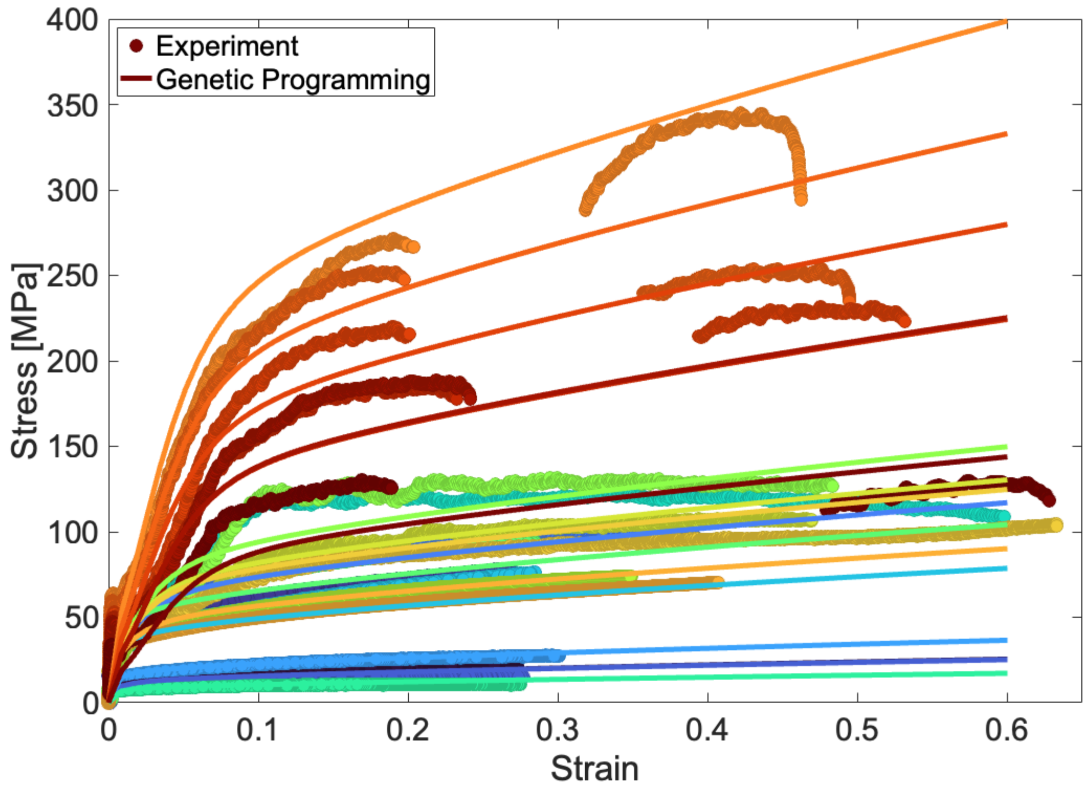
RMSE ~24 MPa



RMSE ~ 14 MPa

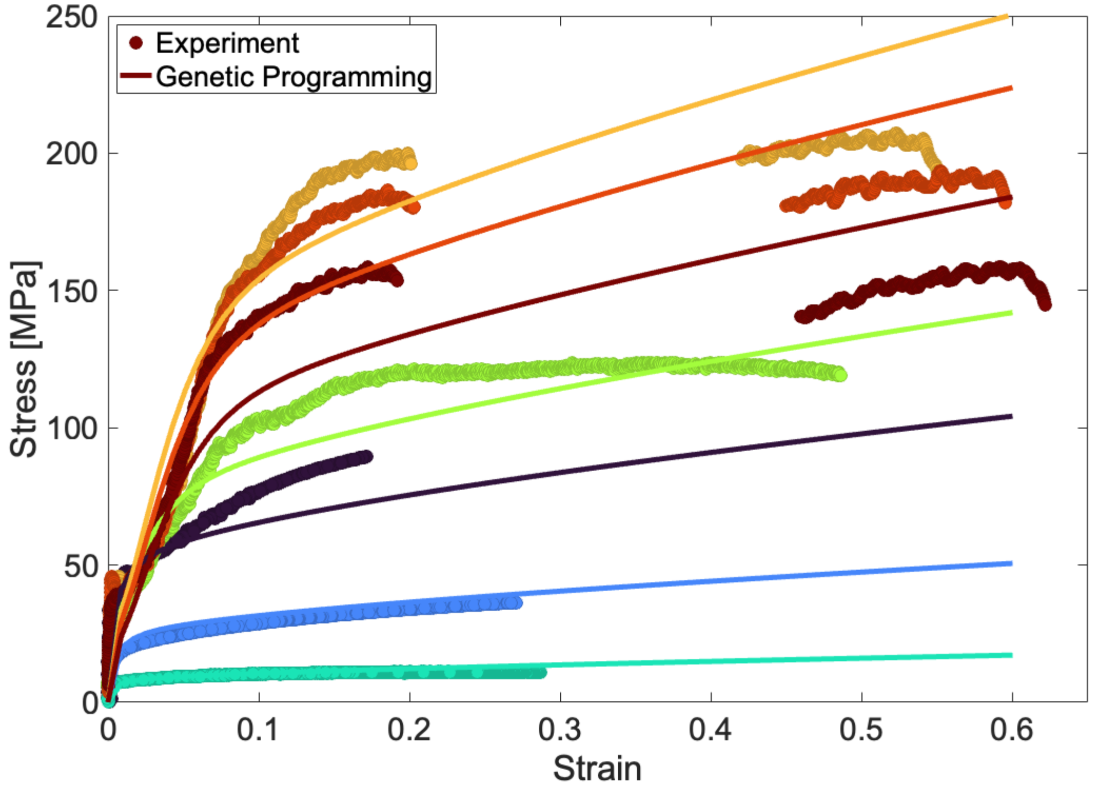
Genetic Programming RMSE Comparison – Training vs. Test

Training set



RMSE ~ 13.32 MPa

Testing set

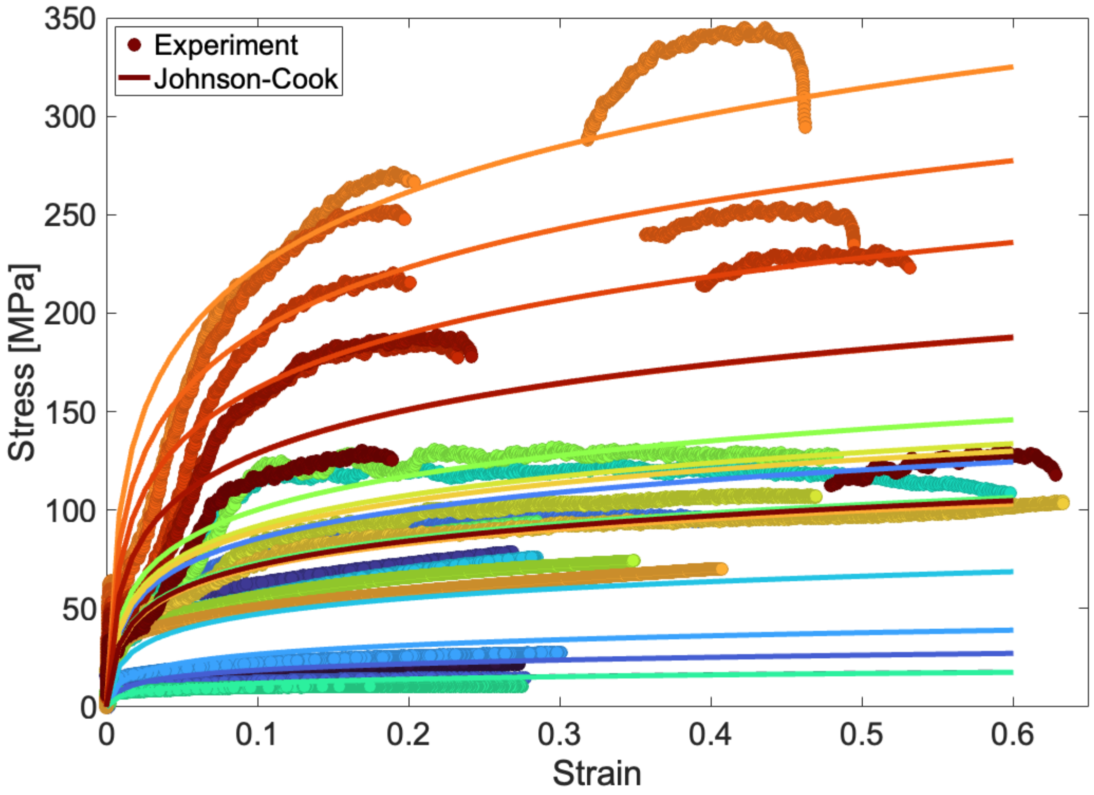


RMSE ~ 13.96 MPa

D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

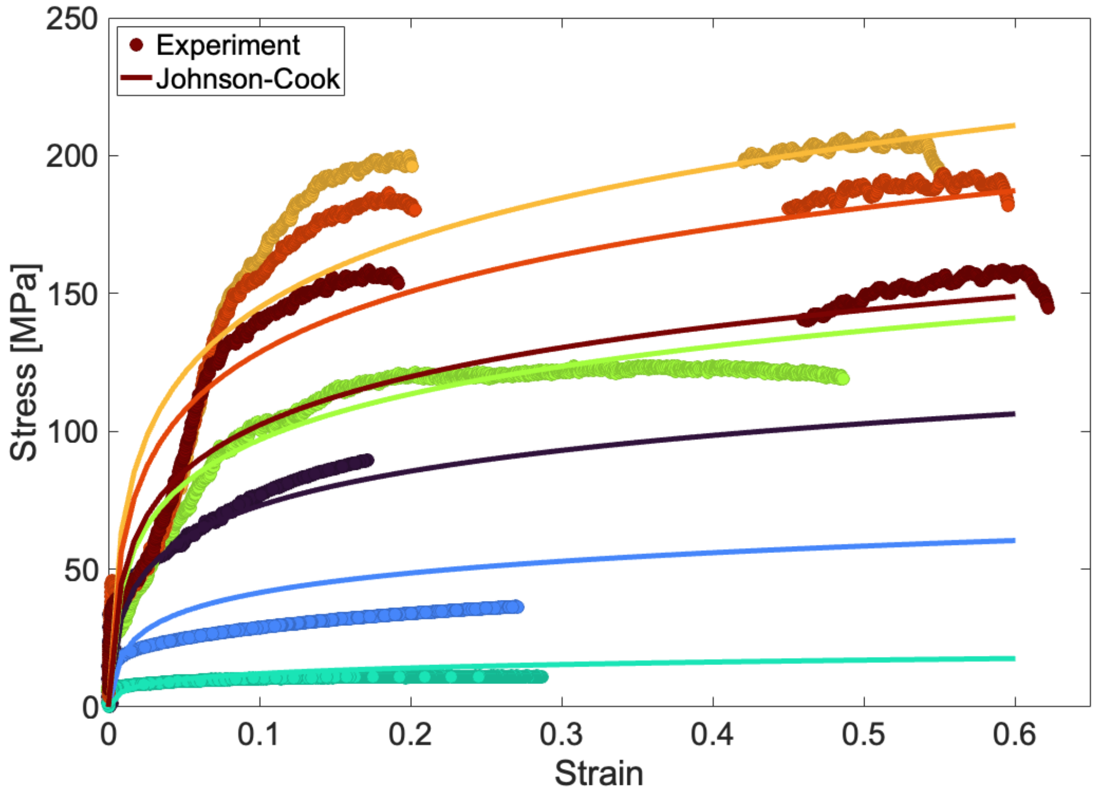
Johnson-Cook RMSE Comparison – Training vs. Test

Training set



RMSE ~ 18.77 MPa

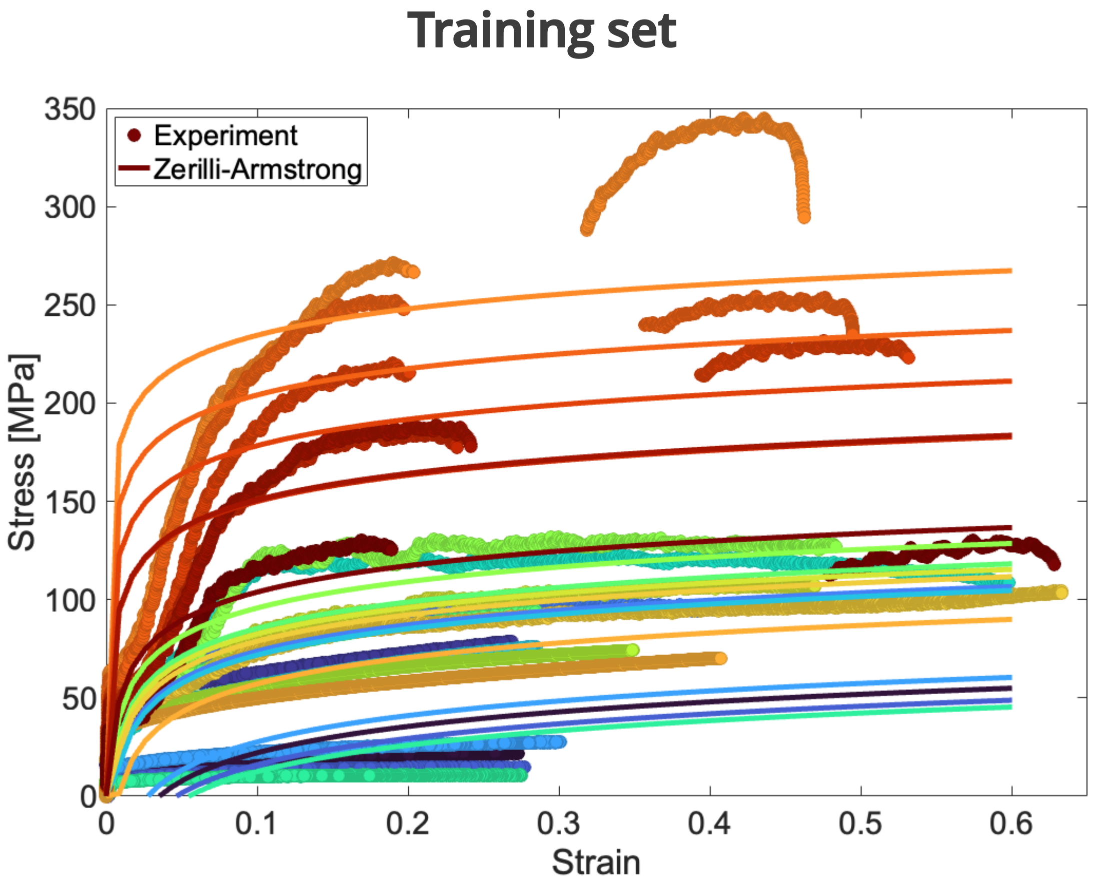
Testing set

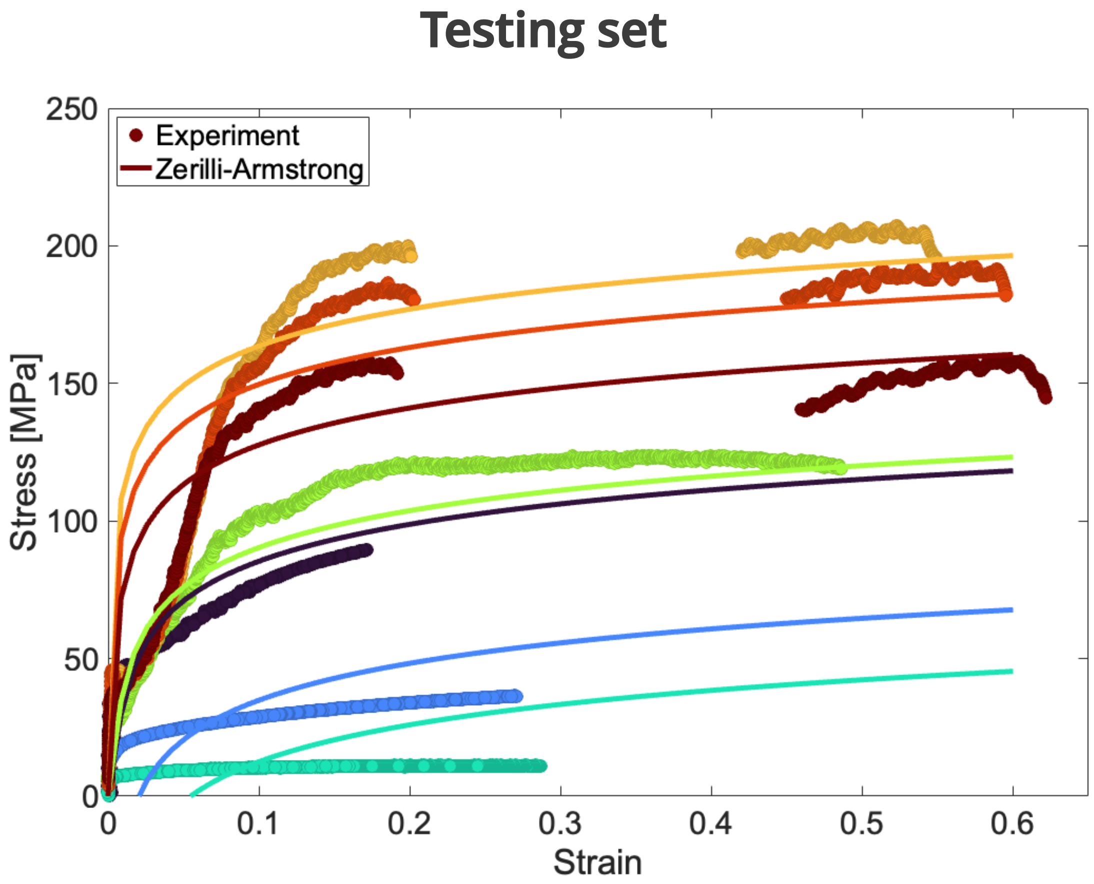


RMSE ~ 19.06 MPa

D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

Zerilli-Armstrong RMSE Comparison – Training vs. Test



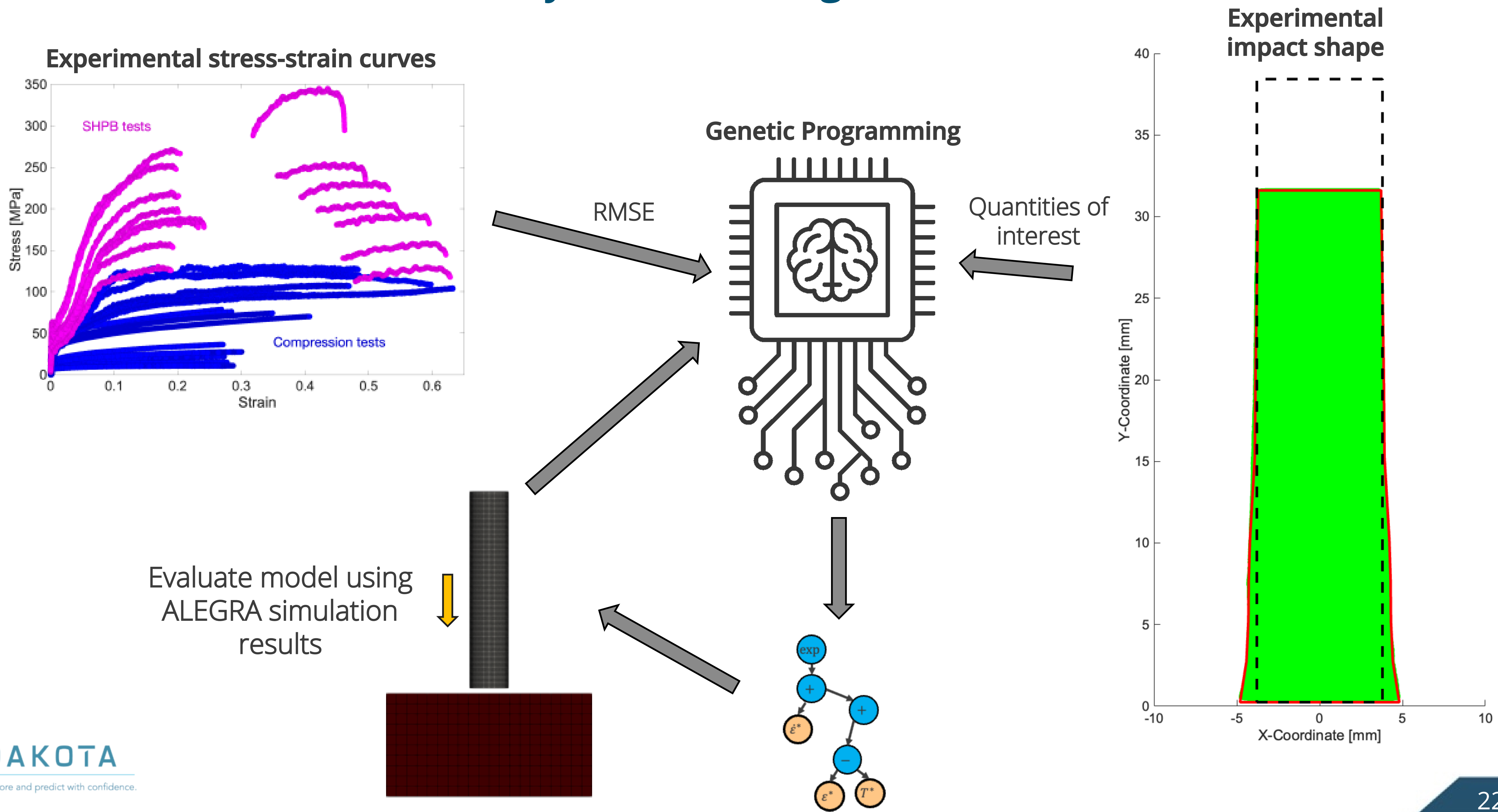


RMSE ~ 24.16 MPa

RMSE ~ 24.03 MPa

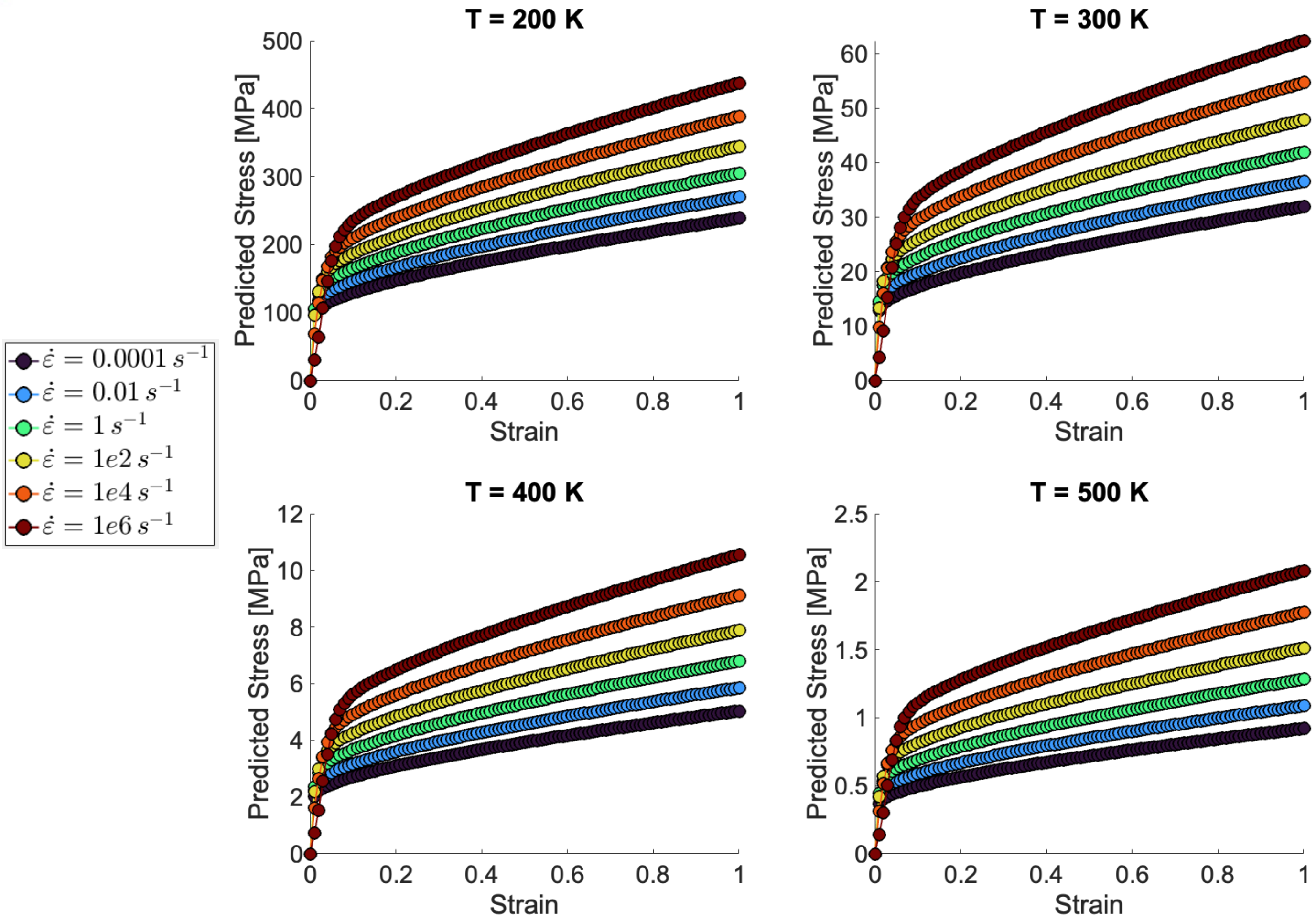
D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

Stress-strain curves may not be enough…

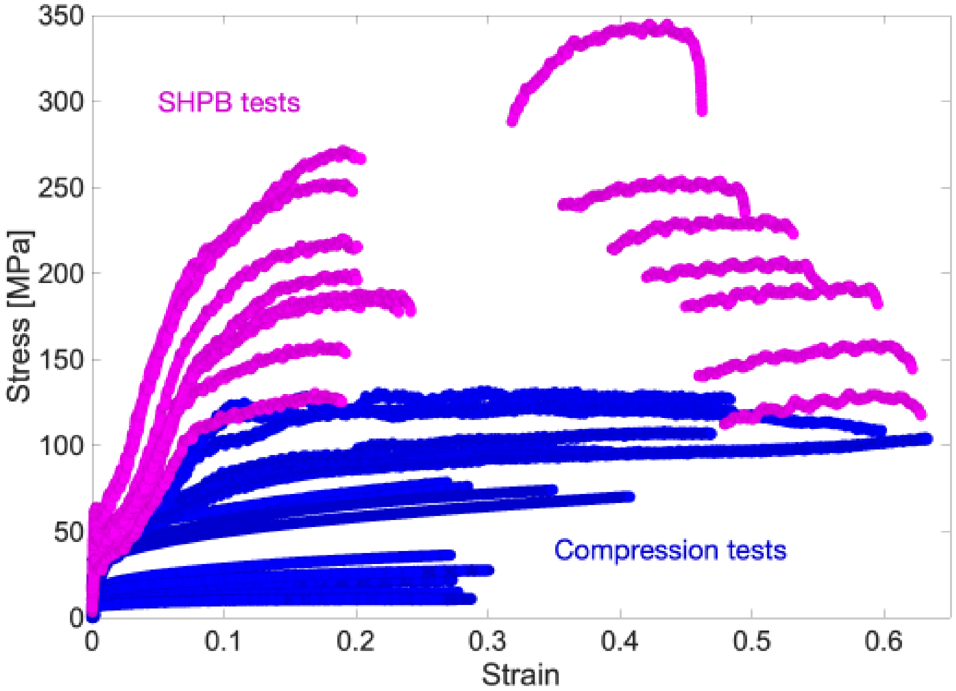


Leveraging the analytical expression

Genetic Programming



Experimental Data



Temperature: $190 \sim 400\ K$

Strain-rate: $0.0001 \sim 3900\ s^{-1}$

H. Lim et al., SAND Report (2022) - SAND2022-2368

Traditional Strength Model Development: **Zerilli-Armstrong and Johnson Cook**

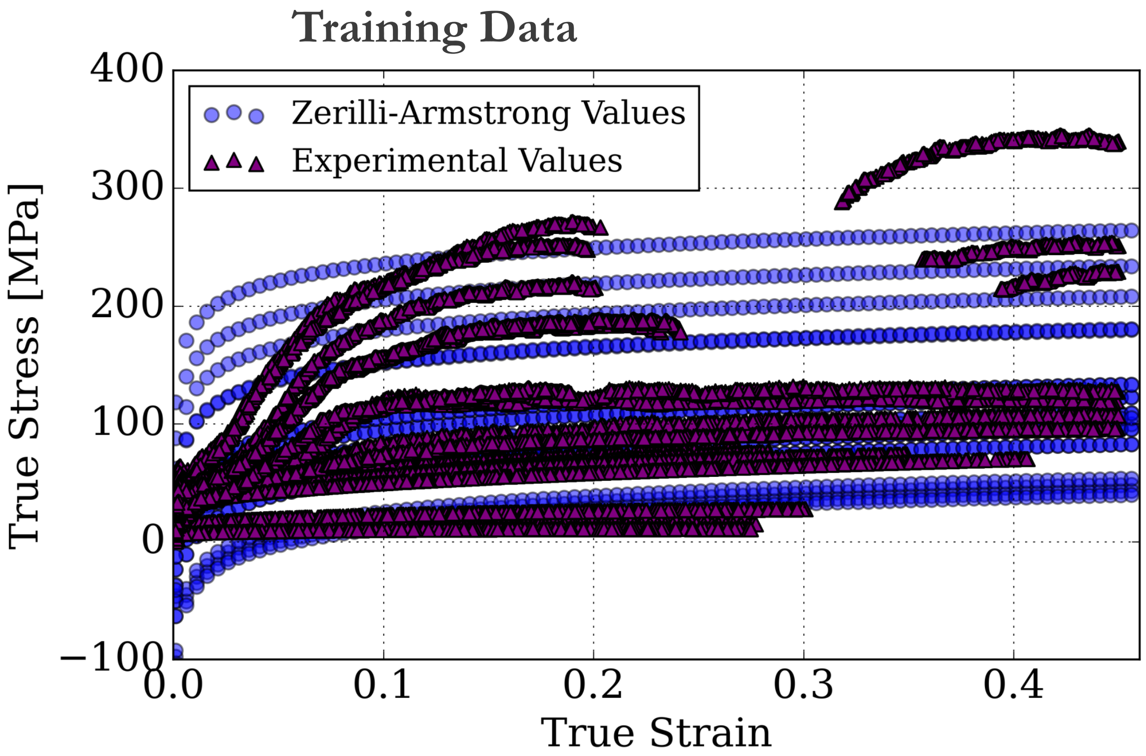
$$\sigma = C_0 + C_1 \exp\left(-C_3 T + C_4 T \ln(\dot{\varepsilon})\right) + C_5 \varepsilon^n$$

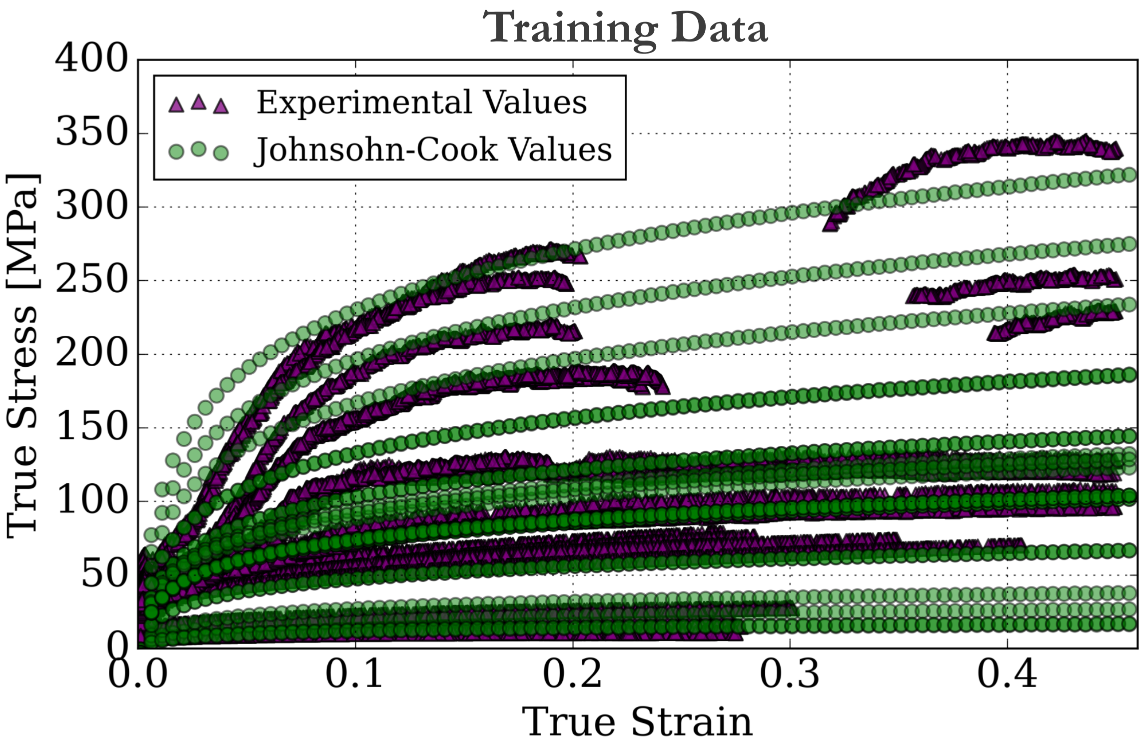
$$\sigma = [A + B\varepsilon^n][1 + C\ln(\dot{\varepsilon})][1 - T^{*m}]$$

$\dot{\epsilon}^* = \dot{\epsilon}/\dot{\epsilon}_0 \quad \dot{\epsilon}_0 = 1\ /s \quad T_m = 505\ K \quad T^* = T/T_m$

C_0 (MPa)	C_1 (MPa)	C_3 (1/K)	C_4 (1/K)	C_5	n
204.98	577.51	0.008	0.0004	−159.08	−0.10

A (MPa)	B (MPa)	n	C	m
−10653.59	15044.97	0.05	0.09	0.05

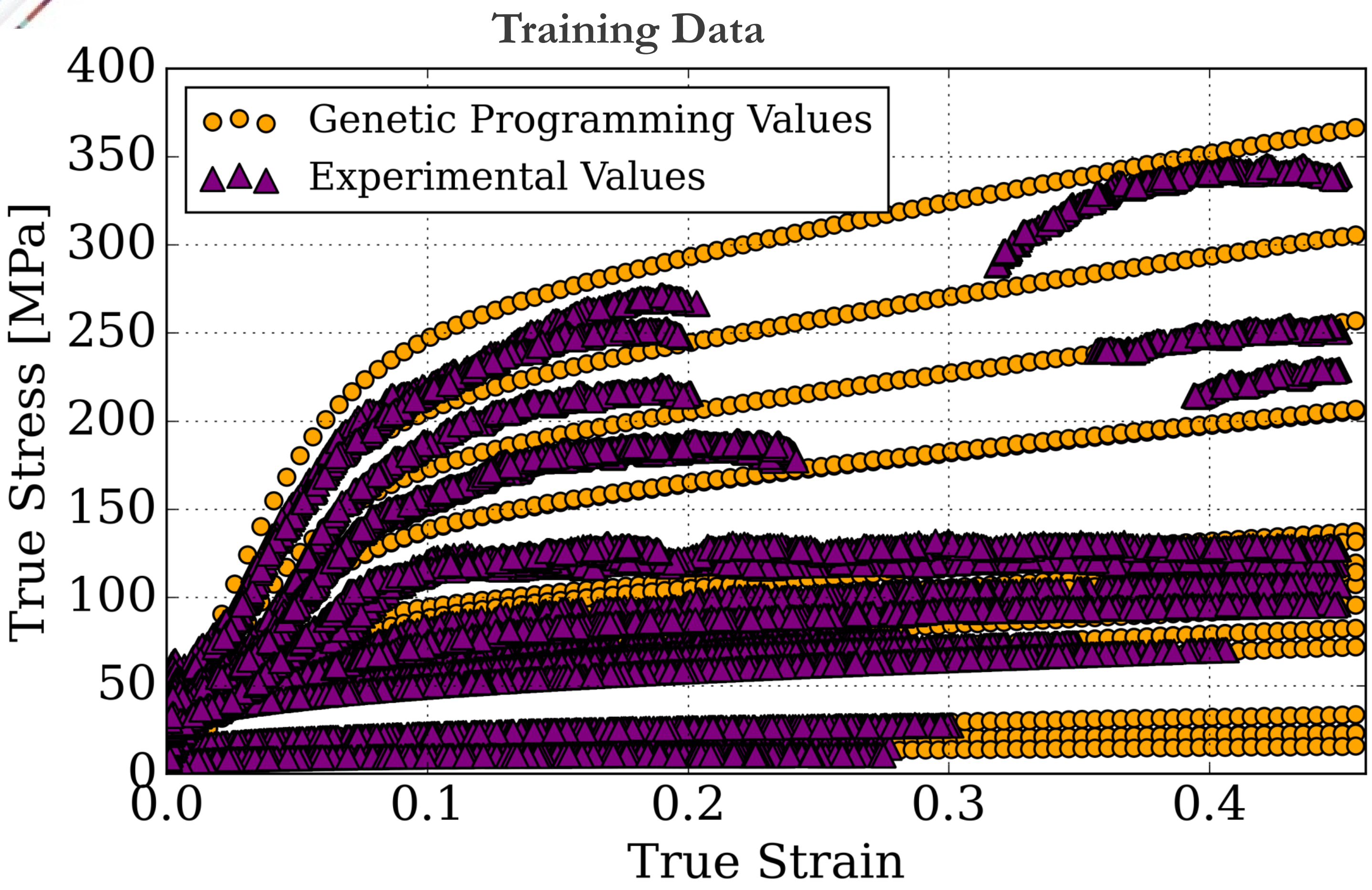


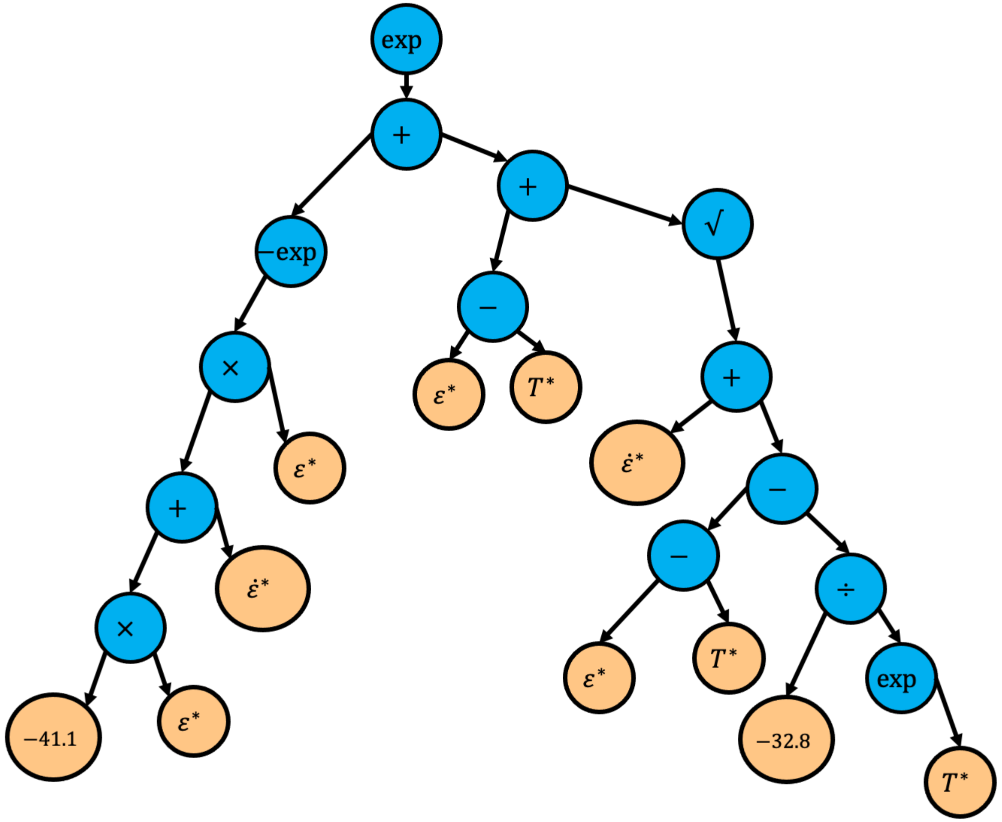


Zerilli et al., (1987) RMSE=24.16 MPa *D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)* RMSE=18.77 MPa Cook et al., (1983)

D. Montes de Oca Zapiain et al., Comp. Mat. Sci. (2023)

Data-driven Strength Model Development: **Best Model**





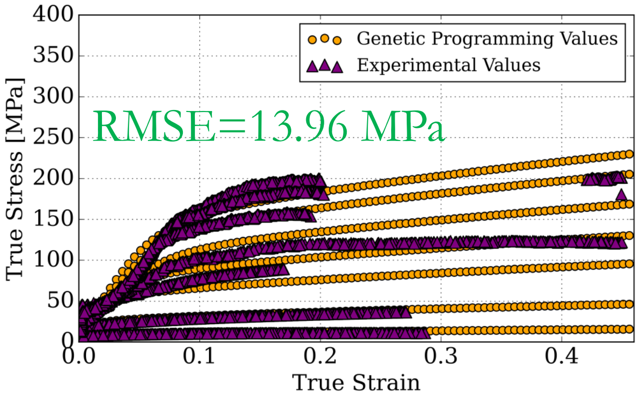
$$\sigma = \exp\left(-\exp\left((-41.1\varepsilon^* + \dot{\varepsilon}^*) * \varepsilon^*\right) + \left((\varepsilon^* - T^*) + \left(\dot{\varepsilon}^* + \left((\varepsilon^* - T^*) - \left(\frac{-32.8}{\exp(T^*)}\right)\right)\right)^{0.5}\right)\right)$$

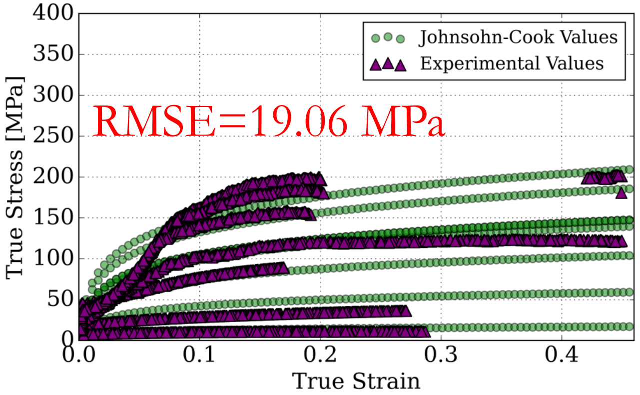
Population=34738 Tournament Size=468 Parsimony Coefficient=0.003

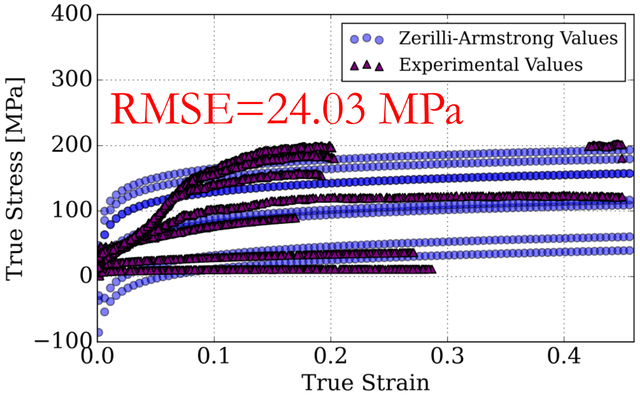
RMSE=13.32 MPa

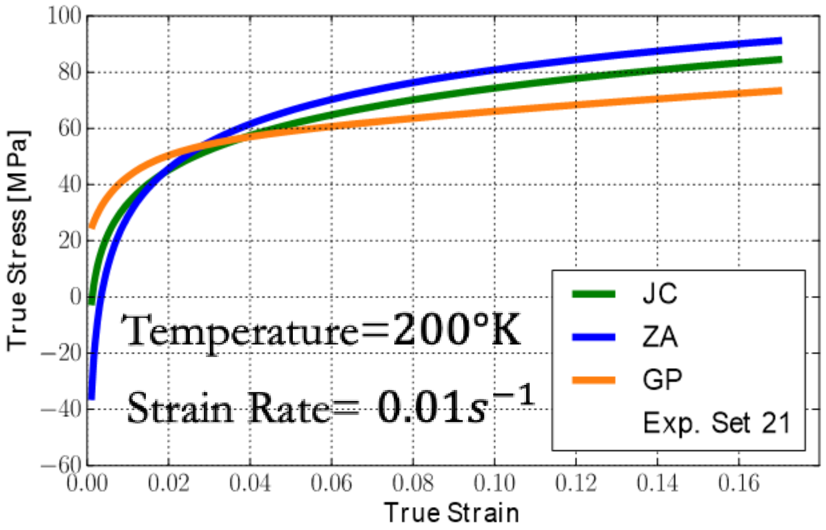
where $\varepsilon^* = \varepsilon^{.396}$ $\dot{\varepsilon}^* = \ln(\dot{\varepsilon})$ $T^* = \frac{T}{T_{melting}}$

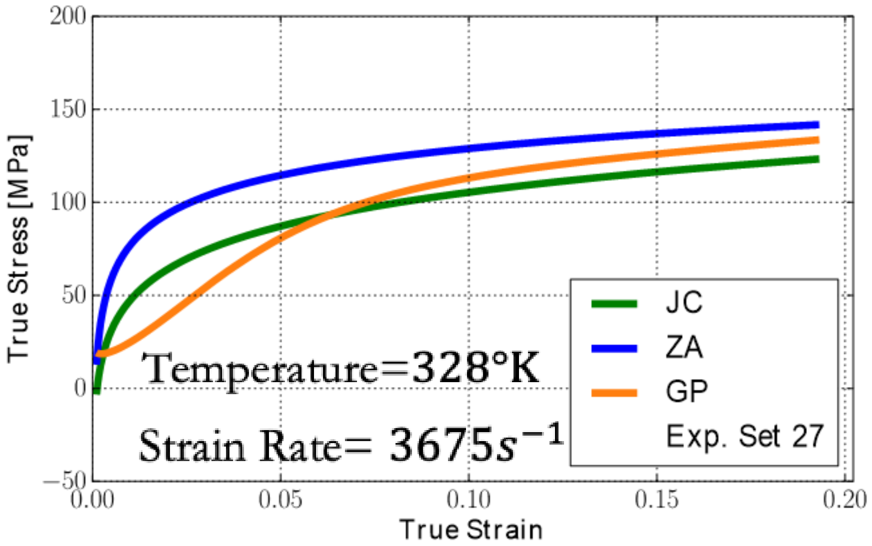
Performance of Different Models: **Evaluation on test set**

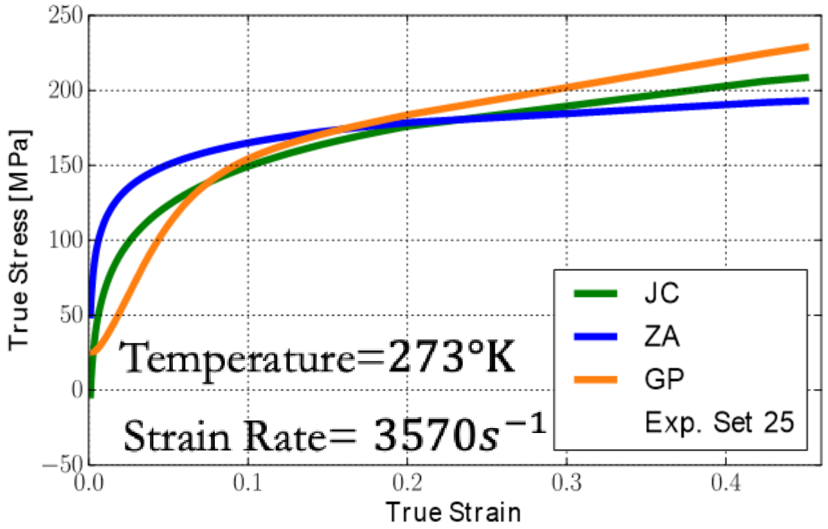












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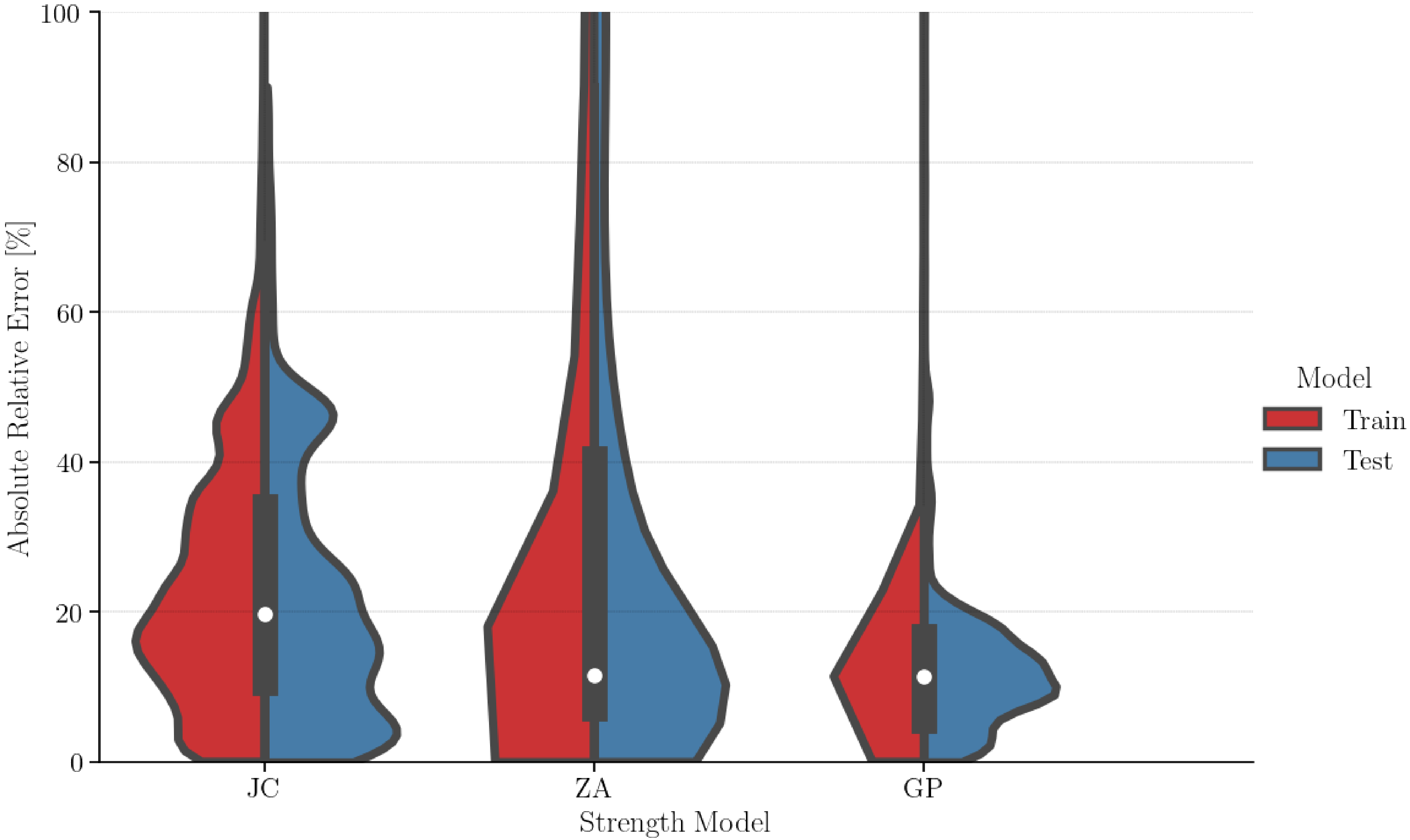
Performance of Different Models: **Traditional vs. GP**



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