Optimizing AI-Enhanced Neural Network Subroutines for Plasticity in FEM

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Advancements in material science and manufacturing processes have revealed the need for custom material models within the Finite Element Method (FEM). While commercial FEM software provides robust frameworks for standard engineering tasks, their limitations become apparent when addressing cutting-edge materials and processes. These challenges are particularly pronounced in modeling materials such as polymers, composites, or advanced alloys, which exhibit behaviors that surpass the capabilities of built-in constitutive models. Traditional FEM tools offer a narrow range of plastic potentials tailored for standard materials like metals. These models typically address isotropic or kinematic hardening but are insufficient for emerging materials. Polymers, composites, and advanced alloys frequently demonstrate complex behaviors [1]

User-defined material subroutines (UMATs) extend FEM capabilities. By allowing engineers and researchers to define unique material responses and incorporate novel mathematical formulations, UMATs address gaps in traditional FEM-based modeling. In implicit time integration FEM codes, UMAT subroutines typically take the strain history as input and compute the updated stress tensor and Jacobian tensor (tangent operator) as outputs. These subroutines enable the implementation of advanced models that include for example new plastic potentials for capturing non-standard material behaviors [2].

The emergence of Artificial Intelligence (AI) offers new computing possibilities. The integration of AI into material modeling introduces a transformative approach to FEM. Specifically, hybrid user subroutines combining physics-based principles with data-driven neural networks (NNs) provide a versatile framework for modeling novel materials. AI predicts parameters challenging to derive analytically, such as strain-dependent evolution of material properties. As is trained with experimental datasets, the neural network ensures full adaptability to emerging material's behavior and guarantees compliance with established mechanical principles [3]. AI substitutes traditional iterative loops in plasticity algorithms, significantly reducing computational costs.

The goal of this research is to propose and validate a methodology for developing an optimized version of an AI-enhanced UMAT, Machine Learning User Material Subroutine (ML-UMAT) applicable to a specific plastic potential. The development and optimization of this hybrid model follow a systematic approach:

- Subroutine development
  - Initial subroutine implementation in Python for neural network development.
  - Transition to Fortran, the typical language used in finite element codes such as ABAQUS [4], ANSYS [5] or CALCULIX [6].
- Neural network design:
  - Dense architecture optimized through hyperparameter tuning.
  - Loss function tailored to subroutine performance metrics, with a custom penalty term to encourage computational efficiency.
- Validation and Performance Testing of:
  - A uniaxial stress state.
  - A complex stress state model with stress concentrations.

The hybrid user subroutine was tested and validated using CALCULIX, an open-source FEM software known for its flexibility, accessibility, and robust features. As a free platform, CALCULIX removes financial barriers, making advanced FEM tools available to a broader audience and fostering innovation and collaboration. Its open-source nature ensures research reproducibility by allowing researchers to share and replicate models and validation cases, enhancing credibility. Furthermore, CALCULIX supports deep customization, enabling the integration of novel material models and hybrid subroutines, essential for advancing experimental methodologies.

The study conducted a comprehensive evaluation of three material subroutines, each representing distinct approaches to modeling plasticity. These subroutines were chosen to highlight the strengths and limitations of both traditional FEM frameworks and the proposed hybrid methodology. Below is a detailed analysis of the three subroutines in order of complexity:

- J2plasticity. This subroutine represents the classic con Mises plasticity model commonly used for metals. It serves as a baseline for evaluating the computational efficiency and accuracy of hybrid models. It provided insights into the performance of traditional plasticity models when applied to standard material behaviors.
- Porous plasticity model. The Gurson-Tvergaard-Needleman (GTN)model extends traditional plasticity by incorporating void nucleation, growth and coalescence, making it suitable for modeling ductile damage in

materials, and tests the hybrid subroutine ability to predict void volume fraction and failure criteria.

- General plasticity. They are designed to handle a wide range of material behaviors, including anisotropy, rate-dependence, and thermo-mechanical coupling. These models often require iterative numerical solutions due to their complexity, and evaluate the hybrid subroutine capability to replicate intricate material responses.

The neural network architecture is a deep fully connected network tailored to replicate the plastic behavior of materials, with the goal of surpassing the computational efficiency of classical material models. The implementation was developed using PyTorch. Hyperparameter optimization was performed using the python library Optuna, which utilized Bayesian optimization to search for the best configuration of hyperparameters, such as the number of layers, neurons per layer, learning rate, and regularization constants.

A distinctive aspect of this optimization process was the inclusion of a custom loss function in the Optuna framework. This loss incorporated a penalty term based on the execution time of the model, encouraging solutions that not only achieved high accuracy but also optimized computational efficiency.

The validation process was conducted using two finite element models. The first model involved a uniaxial tensile test, where a cube was subjected to tensile loading without stress gradients. This simulation served as an initial example to evaluate the fundamental accuracy and stability of the hybrid subroutine and provide a baseline for comparing the neural network predictions against traditional constitutive models. The comparison was carried out by analyzing the computational performance in Python and Fortran environments.

The second validation model, illustrated in Figure 1, consisted of a more complex geometry: a prism with three circular holes subjected to tensile loading. This model introduced stress concentrations, creating a variety of different stress states. The performance of the hybrid subroutine was assessed by benchmarking its execution time and accuracy in CALCULIX, using the UMAT implemented in Fortran. Comparisons were made between the two models and across three plastic potentials: J2, porous plasticity, and a general plasticity model.

In conclusion, the hybrid user subroutine represents a significant advancement in FEM modeling, bridging the gap between traditional physics-based approaches and modern AI-driven methodologies. The hybrid subroutine demonstrated significant improvements in computational efficiency compared to traditional models, while maintaining accuracy. This framework enables the accurate and efficient simulation of complex material behaviors, setting the stage for future innovations in material science and manufacturing.

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Figures

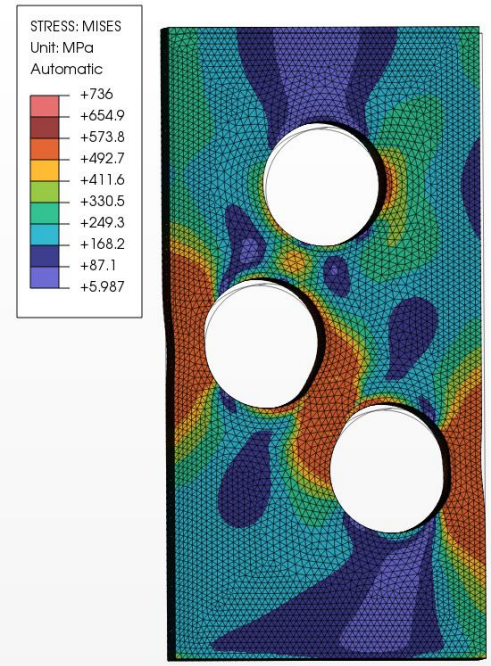

Figure 1. 3D finite element model of a prism with three circular holes used for validation.