ROBUST, CO-DESIGN EXPLORATION OF MULTILEVEL PRODUCT, MATERIAL, AND MANUFACTURING PROCESS SYSTEMS

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ABSTRACT

Achieving targeted product performance requires the integrated exploration of design spaces across multiple levels of decision-making in systems comprising products, materials, and manufacturing processes - Product-Material-Manufacturing Process (PMMP) systems. This demands the capability to co-design PMMP systems, that is, share ranged sets of design solutions among distributed product, material, and manufacturing process designers. PMMP systems are subject to uncertainties in processing, microstructure, and models employed. Facilitating co-design requires support for simultaneously exploring high-dimensional design spaces across multiple levels under uncertainty.

In this paper, we present the ***Co-D****esign* ***E****xploration of* ***M****ultilevel PMMP systems under* ***U****ncertainty (CoDE-MU) framework to facilitate the simultaneous exploration of high-dimensional design spaces across multiple levels under uncertainty. The CoDE-MU framework is a machine learning-enhanced, robust co-design exploration framework that integrates robust, coupled compromise Decision Support Problem (rc-cDSP) construct with interpretable Self-Organizing Maps (iSOM). The framework supports multidisciplinary designers to i) understand the multilevel interactions, ii) identify the process mechanisms that affect material and product responses, and iii) provide decision support for problems involving many goals with different behaviors across multiple levels and uncertainty.*

We use an industry-inspired hot rod rolling (HRR) steel manufacturing process chain problem to showcase the CoDE-MU framework's efficacy in facilitating the simultaneous exploration of the product, material, and manufacturing process design spaces across multiple levels under uncertainty. The framework is generic and facilitates the co-design of multilevel PMMP systems characterized by hierarchical product-material-manufacturing process relations and many goals with different behaviors that must be realized simultaneously at individual levels.

Keywords: Co-design, Robust design, coupled-compromise Decision Support Problem (c-cDSP) construct, interpretable Self-Organizing Map (iSOM)

GLOSSARY

Product-Material-Manufacturing Process (PMMP) system: We define PMMP systems as systems comprising the product, its materials, and associated manufacturing processes.

Design Level: We define 'design level' as the interface where design decisions are made by disciplinary experts regarding products, materials, and manufacturing processing, considering their interactions. The disciplinary experts correspond to the product, materials, and process designers, respectively.

Robust satisficing solutions: Solutions that are relatively insensitive to uncertainties and satisfice the designer's requirements.

Co-design: We define co-design from an ICME perspective as a design that supports distributed disciplinary experts, such as product, material, and process designers, across multiple levels of decision-making to work collaboratively in ensuring PMMP system performance. In co-design, designers are supported in i) making decisions simultaneously across multiple levels while considering their interrelations and ii) managing design conflicts to ensure collaboration.

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Robust Co-design: We define robust co-design from an ICME perspective as a co-design that supports designers across multiple levels to manage inherent uncertainties by facilitating the identification of a ranged set of common robust satisficing solutions across the levels.

NOMENCLATURE AND LIST OF SYMBOLS

[C]	- Carbon concentration
c-cDSP	- coupled-compromise Decision Support Problem
cDSP	- compromise Decision Support Problem
C_{eq}	- Equivalent Carbon
CoDE-MU	- Co-Design Exploration of Multilevel PMMP systems under Uncertainty
CR	- Cooling Rate
[Cu]	- Copper concentration
DBD	- Decision-Based Design
DCI	- Design Capability Index
DSIDES	- Decision Support In the Design of Engineering Systems
DSP	- Decision Support Problem
D_α	- Ferrite Grain Size
d_γ	- Austenite Grain Size
EMI	- Error Margin Index
GoID	- Goal-oriented Inverse Design
HRR	- Hot Rod Rolling
HV	- Hardness
ICME	- Integrated Computational Materials Engineering
IDEM	- Inductive Design Exploration Method
iSOM	- interpretable Self-Organizing Map
[Mn] and [Mn_{copy}]	- Manganese concentration
MDO	- Multi-Disciplinary Optimization
[N]	- Nitrogen concentration
p	- Pearlite colony size
[P]	- Phosphorus Concentration
PMMP	- Product, Material, and Manufacturing Process
PSPP	- Processing-microStructure-Property-Performance
rc-cDSP	- robust, coupled-compromise Decision Support Problem
SOM	- Self-Organizing Maps
[Si]	- Silicon concentration
S_0	- Pearlite interlamellar spacing
t_{carb}	- Carbide thickness
T_{mf}	- Average Austenite to Ferrite transition temperature
TS	- Tensile Strength
X_f	- Ferrite fraction
$X_{f\,eq}$	- Equivalent Ferrite fraction
YS	- Yield Strength
ε_r	- Residual strain at the end of rolling

1. FRAME OF REFERENCE

The achievement of targeted product performance requires careful consideration of the relations among products, their materials with respective microstructures, and associated manufacturing processing. Product performances are defined by many property requirements with different behaviors that need to be realized simultaneously. The manufacture of steel rods through the hot rod rolling (HRR) manufacturing process chain [1] is an example that illustrates the relations among manufacturing processing, material microstructure, and product properties and performance. In the HRR of steel, cast steel billets are reheated and subsequently processed in rolling and cooling mills to produce hot-rolled steel rods as products. The mechanical properties of the hot-rolled steel rods identify their performance. The steel microstructure determines the mechanical properties. The steel microstructure is influenced by the thermo-mechanical processing that steel billets undergo. Given the relations among manufacturing processing, material microstructure, and product properties and performance, realizing targeted product performance requires a collective consideration of a system comprising the products, materials, and manufacturing processes [2], referred to as *Product-Material-Manufacturing Process (PMMP) systems* in this paper. This necessitates an integrated, top-down, systems-based approach for designing PMMP systems, starting with the property requirements and inversely designing the material microstructure and processing paths to realize the targeted product performance [3]. Olson's Processing-microStructure-Property-Performance (PSPP) relations [4] lay the foundation for the inverse, systems-based design of PMMP systems by connecting the product, materials, and manufacturing processes, as depicted in Figure 1. According to the PSPP relations, the processing during manufacturing determines the material microstructure and properties, which in turn determines the product properties and performance.

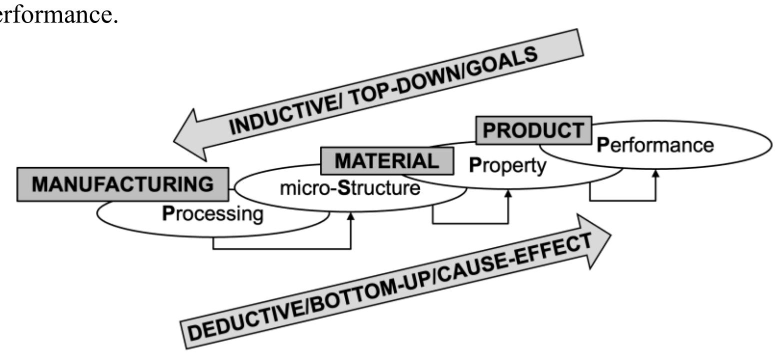

FIGURE 1. Olson's Processing-microStructure-Property-Performance (PSPP) relations [4] that connect products, materials, and manufacturing processes.

The design of PMMP systems involves decision-making by different disciplinary experts, such as product, material, and process designers. The expert decisions are made across multiple levels of a decision hierarchy defined based on the PSPP relations. The decisions at individual levels in the PMMP system are directed toward simultaneously achieving their design goals with different behaviors. The difference in behaviors necessitates the trade-offs or compromises among the goals. Individual-level decisions require careful consideration of the level-specific constraints and design variable bounds. The individual-level decisions collectively determine product performance. Due to their interrelations, decisions at an individual level will affect the decisions at another interrelated level, impacting product performance. Individual-level decisions can result in ' design conflicts when made in isolation without considering their interrelations.' We consider design conflicts as situations where the goal-directed decisions at an individual level do not align with the goal-directed decisions at another interrelated level. Design conflicts will result in poor PMMP system performance and products not meeting targeted performance requirements. In this paper, we focus on the simulation-supported design of PMMP systems that help reduce dependency on expensive and time-consuming lab-scale experimentation and plant trials [5]. The Integrated Computational Materials Engineering (ICME) initiative [6] provides a heading for simulation-supported PMMP systems design. ICME focuses on the simulation-supported, concurrent, top-down design of products and materials by using the PSPP relations to link materials models across multiple length and time scales. According to McDowell [7], simulation-supported systems design approaches should enhance the designer's understanding of complex relations in the system to help make informed decisions. The decisions in simulation-supported PMMP system design are based on simulation-generated information. In simulations, designers use models that are incomplete, inaccurate, and abstractions of underlying physical phenomena [8] and therefore, they embody uncertainty. The decisions at individual levels are also subject to design variable uncertainties arising from random variations in manufacturing processing and material microstructure. These inherent uncertainties adversely impact the decisions at individual levels and PMMP system performance. Therefore, the simulation-supported integrated design of PMMP systems requires support for i) consideration of the relations among individual-level decisions, ii) management of design conflicts, and iii) management of uncertainties. This necessitates the facilitation of 'robust co-design,' allowing designers distributed across multiple levels to collaborate by supporting i) the consideration of the relations among individual-level decisions and ii) the management of uncertainties and design conflicts. By facilitating collaboration, the satisfaction of the level-specific design goals and the PMMP system performance under conditions of uncertainty is ensured. Collaboration is achieved by supporting 'co-design exploration' - the simultaneous exploration of the multilevel design spaces to identify a ranged set of common 'robust satisficing solutions' across levels. Robust satisficing solutions are relatively insensitive to uncertainties and 'satisfy' and 'suffice' the design requirements.

From a systems design perspective, we consider design a goal-oriented, decision-based process supported by simulations. Therefore, we abide by the Decision-Based Design (DBD) paradigm advocated by Mistree and co-authors [9], where designing is considered a decision-making process wherein designers make a series of decisions, some sequentially while others concurrently. The decisions in DBD are modeled using the Decision Support Problem (DSP) technique [9], anchored in the notion of bounded rationality proposed by Herbert A. Simon [10]. The information required to support decisions in DBD is generated using empirical or simulation-driven surrogate models that are abstractions of reality. Therefore, we seek a ranged set of '*satisficing solutions*' [11] that 'satisfy' and 'suffice' the designer's requirements for the many goals of the design problem by exploring the solution space. The use of the compromise Decision Support Problem (cDSP) [12] construct supports exploring satisficing solutions for problems involving many goals with different behaviors, where goal trade-off considerations are essential. Using the coupled cDSP (c-cDSP) construct [13], designers can model interrelated decision problems across multiple levels, with decisions at individual levels requiring trade-offs among the many goals. The design spaces generated by executing the DSP are explored to identify a '*ranged set of satisficing solutions.*' The ranged set of satisficing solutions helps designers identify i) regions of interest in the design space that require further detailed exploration and ii) key design variables and important relations in a system. In this paper, we look at managing uncertainties by designing the system to be relatively insensitive to uncertainties without reducing or eliminating them, termed 'robust design.' Unlike uncertainty mitigation approaches that involve developing 'perfect' models by collecting more data and performing extensive computations to quantify uncertainties, uncertainty management is computationally less expensive. Uncertainty management is achieved by seeking 'robust solutions' that are relatively insensitive to uncertainties. Type I, Type II, and Type III robust designs are discussed in the literature [1] to deal with uncertainties associated with random noise, design variables, and models, respectively. The use of the Design Capability Index (DCI) [14] and Error Margin Index (EMI) [15] robust design indices in conjunction with the DSP construct have been proposed to help identify a ranged set of '*robust satisficing solutions*' for Type I and II robust designs, and Type III robust design, respectively.

Most current approaches discussed in the literature for the top-down design of PMMP systems are sequential. Adams and co-authors [16] present a framework to support the inverse design of systems involving materials and processes by employing spectral representation to establish invertible relationships between the same. The materials knowledge systems approach is presented by Kalidindi and co-authors [17, 18], where the bi-directional information flow between different length scales is facilitated to support inverse materials design. Ghosh and co-author [19] present a scalable framework for explicit inverse design named probabilistic machine learning for inverse design. The explicit inverse design is modeled in the framework using a conditional invertible neural network. The focus here is on supporting the identification of product designs that meet targeted performance. This is demonstrated in the inverse aerodynamic design of three-dimensional turbine blades. Sui and co-authors [20] present a deep reinforcement learning scheme for automating the inverse design of composite material structures to realize the required properties. The scheme is applied to a two-dimensional composite planar structure design problem to achieve the strongest average structure tensile strength along the primary axes. Chen and co-authors [21] present a machine-learning-based inverse materials design approach that combines generative inverse design networks, backpropagation, and an active learning strategy to support composite materials design. Kumar and co-authors [22] propose a machine learning-based inverse design technique using neural networks to realize metamaterials with desired properties by tailoring the material topologies. Tsai and co-authors [23] and Qian and co-authors [24] present inverse design approaches that combine artificial neural networks and the genetic algorithm to relate processing with product properties and material properties with structure, respectively. The sequential nature of these approaches results in isolated decision-making across individual levels, thereby failing to consider the multilevel relations and resulting in design conflicts that impact the PMMP system performance. The use of multidisciplinary optimization (MDO) [25] approaches, such as analytical target cascading [26], collaborative optimization [27], and bilevel integrated system synthesis [28, 29] for optimizing multilevel systems while considering the multilevel interactions are discussed in the literature. Ituarte and co-authors [30] present a computer-aided expert system where MDO and surrogate models are employed to conduct trade-off exploration and optimization by coupling product design, materials systems, and manufacturing processes. The authors demonstrate the exploration of optimized solutions across the product, material, and manufacturing disciplines for a digital manufacturing scenario to ensure overall system performance. Rigorous and iteratively intensive optimization techniques that involve optimization loops within and between levels are employed in MDO approaches to identify unique single-point solutions at each level. This is especially challenging during design exploration, where the focus is on quickly identifying a set of satisfactory solutions instead of a unique single-point solution [31]. In the optimization formulation employed in MDO approaches, designers assume the perfectness of the models and objective function and the availability of all required information. Given that the models used are abstractions of reality, the objective functions are imperfect, and the information available is incomplete, our focus is on 'satisficing' rather than 'optimizing.' We therefore seek a ranged set of robust satisficing solutions.

Different approaches that support multilevel co-design exploration under uncertainty by identifying robust satisficing solution sets have been discussed in the literature. Choi and co-authors [3] propose the Inductive Design Exploration Method (IDEM) to support the robust co-design of multilevel systems. IDEM involves sequentially identifying and propagating a range of robust solutions among the individual levels. IDEM is limited by the number of design variables that can be considered, discretization errors, increased computational expense for improved accuracy, and limited flexibility in design, as discussed in [1]. Nellippallil and co-authors [1] present an inverse robust design approach named Goal-oriented Inverse Design (GoID) to address some of the limitations in IDEM and support the co-design of systems composed of hierarchically connected products, materials, and associated manufacturing processes. The GoID approach supports sequential design space exploration at the individual levels to identify robust satisficing solutions and their propagation as targets inversely along the hierarchical process chain. The GoID approach does not support the management of design conflicts that can arise due to the sequential nature of design space exploration. To address this shortcoming, Baby and Nellippallil [32] present an information-decision framework to support the systematic detection and management of design conflicts. This is achieved by controlling the design space and decisions across different levels of decisions made sequentially. The IDEM, GoID approach, and the information-decision framework presented by Baby and Nellippallil do not support the simultaneous exploration of the individual levels.

Our focus in this paper is on providing decision support during the simulation-supported design of multilevel PMMP systems under uncertainty. From a DBD perspective, we hypothesize that this can be achieved by facilitating robust co-design using a decision support framework that supports i) modeling the level-specific decision problems and their interactions with other levels in PMMP systems in terms of the flow of information, ii) consideration of uncertainties in the decision problems, and iii) co-design exploration of the multilevel design spaces to identify common robust satisficing solutions and thereby manage design conflicts. Given the many design goals at individual levels that require trade-offs and the interactions of decisions across levels, we model the individual-level decision problems and their interaction in PMMP systems using the c-cDSP construct discussed in Section 3.1.1. A combination of Preemptive and Archimedean formulations is used in the c-cDSP. Using the Preemptive formulation, designers can consider the interrelations among the decision problems across multiple levels of a decision problem. Using the Archimedean formulation, designers can consider many goals that require trade-offs at individual levels of a multilevel decision problem. By combining the two, designers can use a coupled DSP formulation to account for many design goals at individual levels and hierarchical relations across levels of a multilevel decision problem. The EMI and DCI robust design indices presented in Section 3.1.2 are combined with the c-cDSP construct to establish the robust, coupled cDSP (rc-cDSP) that helps designers generate robust design solutions across multiple levels. The design spaces across the multiple levels in the PMMP system are visualized in an integrated manner using the interpretable Self Organizing Maps (iSOM) [33] discussed in Section 3.1.3. The integrated iSOM visualization facilitates co-design exploration to identify common robust satisficing solution sets across multiple levels. In this paper, we present the **Co**-**D**esign **E**xploration of **M**ultilevel PMMP systems under **U**ncertainty (CoDE-MU) framework that enables designers to i) model decision problems at individual levels and their interactions, ii) consider uncertainties, and iii) visualize and efficiently explore multilevel design spaces simultaneously to support robust co-design. The CoDE-MU framework's novelty lies in two aspects: a) support for modeling multilevel design problems characterized by the need to consider trade-offs among many goals at individual levels and interactions across levels, using a coupled decision problem formulation. This is achieved by combining the Preemptive and Archimedean formulations in the c-cDSP; b) support for the joint management of design conflicts and uncertainties across multiple levels through co-design exploration. Co-design exploration involves the simultaneous exploration of multilevel design spaces. It is realized by exploiting the inherent interpretability and correlated nature of the iSOM plots to help designers efficiently identify common robust satisficing solutions.

A description of the problem is presented in Section 2. In Section 3, the CoDE-MU framework to support the robust co-design exploration of multilevel PMMP systems is presented. In Section 4, we showcase the framework's efficacy in supporting the simultaneous exploration of design spaces across multiple levels in PMMP systems and managing uncertainties using an industry-inspired steel manufacturing process chain test problem – the HRR of steel. In the HRR problem, we focus on the interactions between the material and cooling process designers at different levels. We end the paper with our key findings and closing remarks in Section 5. In Appendix A, we present the empirical models that relate the design variables and goals in the coupled HRR problem.

2. PROBLEM DESCRIPTION: ACCOUNTING FOR INTERACTIONS ACROSS MULTIPLE LEVELS AND UNCERTAINTIES INVOLVED IN THE DESIGN OF PMMP SYSTEMS

The design of PMMP systems involves decisions by the product, materials, and process designers regarding the product, its materials, and associated manufacturing processes, respectively. The product designer makes decisions regarding the properties that define the product performance; the materials designer makes decisions regarding material microstructure and composition that defines material properties; and process designers make decisions regarding material processing and input material characteristics that determine the end of processing material microstructure. The interrelated decisions are made across multiple design levels in a design hierarchy defined by the PSPP relations, as depicted in Figure 2.

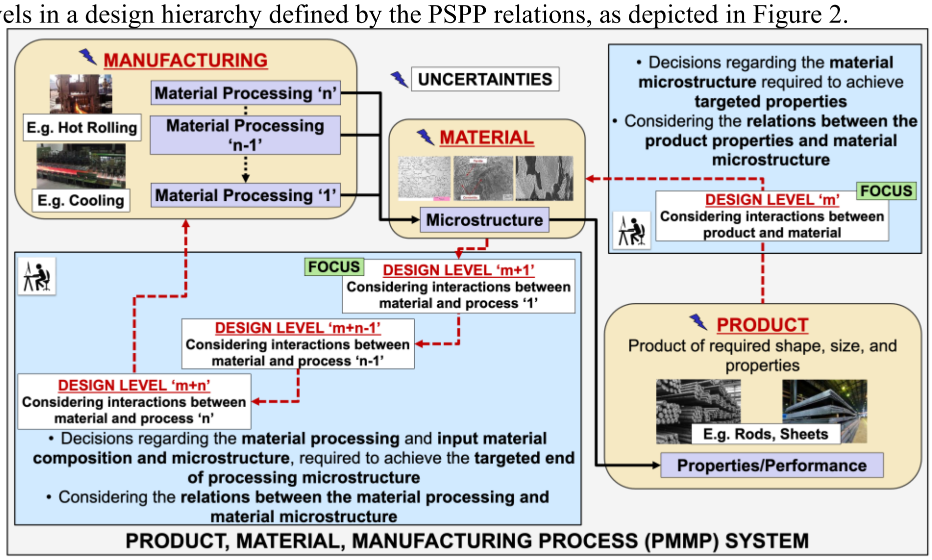

FIGURE 2: Design of PMMP system: Multilevel nature of the PMMP system considering the multiple levels of decisions, multilevel interactions, and uncertainties across the multiple levels. The black arrows depict the forward flow of material, and the red dashed arrows represent the inverse flow of information across multiple design levels that connect the manufacturing processing, material, and product.

In Figure 2, Design Level 'm' involves decisions by the materials designer at the top of the hierarchy, followed by the various process designer's decisions across Design Levels 'm+1' to 'm+n.' Design Levels 'm+1' to 'm+n' are related to the corresponding material processing '1' to 'n' during manufacturing. In this paper, for demonstration purposes, we focus on the interactions between the Design Levels 'm' and 'm+1' of the design hierarchy, where m = 1. At Design Level 'm' or '1'- the upper level, decisions are made regarding the material microstructure required to achieve targeted properties by considering the relations between the product properties and material microstructure. At the lower level - Design Level 'm+1' or '2', decisions are made regarding the input material composition and microstructure and the processing during manufacturing process '1' required to achieve the targeted microstructure. This requires considering the relations between the material processing '1' and the material microstructure. Decisions at Design Level 1 will influence the decisions at Design Level 2. Sequential decision-making across the individual levels in an isolated manner will result in design conflict, where decisions at Design Level 1 regarding the material microstructure required to achieve the targeted property goal values may not be achievable at Design Level 2, given the resource constraints. Resource constraints at Design Level 2 are defined in terms of process limitations and compositional or microstructural characteristics of the input material. The design conflict will result in targeted product performance not being achieved. Hence, the collective consideration of the decisions across the individual levels is vital to account for their interactions and manage design conflicts, thereby ensuring targeted product performance during PMMP systems design. This necessitates co-designing the individual levels, where designers at different levels are supported in identifying and sharing ranged sets of design solutions across the levels. Co-design requires support for simultaneously exploring the design spaces across the individual levels. The decisions at the individual levels are subject to various uncertainties associated with the models employed and other random variations stemming from manufacturing processing and material microstructure. Therefore, management of these uncertainties during PMMP systems design is also essential. This can be achieved by facilitating the identification of *robust satisficing solutions*. In this paper, we specifically focus on uncertainties associated with the design variables and models. Overall, the need in designing PMMP systems is the support for *simultaneous multilevel design exploration to identify a ranged set of common robust satisficing solutions* across multiple levels.

3. A FRAMEWORK TO FACILITATE ROBUST CO-DESIGN EXPLORATION OF MULTILEVEL PMMP SYSTEMS

In this section, we present a framework, namely Co-Design Exploration of Multilevel PMMP systems under Uncertainty (CoDE-MU), that supports designers in simultaneously exploring design spaces across multiple levels to identify a ranged set of common robust satisficing solutions. Using the CoDE-MU framework, we facilitate the co-design of multilevel PMMP systems that involve the product, materials, and manufacturing processes while considering the uncertainties. We begin this section by discussing the various constructs and tools employed in the framework. This is followed by a discussion on decision support using the framework.

3.1. Constructs and tools used in the CoDE-MU framework

Three primary constructs and tools are employed in the CoDE-MU framework. They are i) the coupled-cDSP (c-cDSP) construct, ii) Robust design constructs – DCI and EMI, and iii) the iSOM visualization tool. A discussion of the constructs and tools follows.

3.1.1. c-cDSP construct

The coupled DSP [13] is a DSP construct that supports designers to account for the relations among decisions made hierarchically or concurrently across multiple levels. Using the coupled DSP construct, the relations among the decisions at different levels are modeled as either a vertical or horizontal coupling [13]. Vertical coupling is used for hierarchical decisions, and horizontal coupling is used for concurrent decisions. Decisions at individual levels are directed towards simultaneously meeting many design goals with different behaviors, requiring trade-offs to be made. Hence, we use a c-cDSP to model the multilevel decisions and their relations in PMMP systems. In c-cDSPs, the level-specific information regarding design variables, design goals, and constraints is captured using the keywords – *Given, Find,* and *Satisfy*, as depicted in Figure 3. Figure 3 depicts the basic structure of the c-cDSP for a system with two levels, Design Levels 1 and 2.

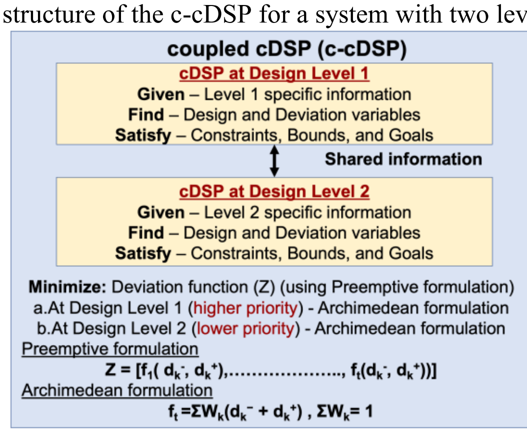

FIGURE 3: The basic structure of the coupled cDSP (c-cDSP) construct

The focus in utilizing the c-cDSP is to find solutions that *minimize* the total deviation of all the design goals in the system from their target values, termed the *'deviation function.'* Based on the coupling between the individual levels, the deviation function in c-cDSPs is modeled using a combination of Preemptive and Archimedean formulations. Using the Preemptive formulation, designers can consider the relations among decisions made sequentially across multiple levels of a decision hierarchy. Since the decisions in PMMP systems are made sequentially across different levels of a decision hierarchy defined by the PSPP relations, the Preemptive formulation is used to model the relations across design levels. In the preemptive formulation, the goals at different design levels are ordered into different priority sets, as depicted in Figure 3. The priority sets are ordered according to the position of the design level in the decision hierarchy. The design goals are satisfied in the order of priority sets, with goals at a higher priority set being met first before meeting the goals at a lower priority set [12]. The use of the Preemptive formulation, therefore, allows designers to i) consider the relations among decisions made sequentially across different levels of a decision hierarchy and ii) assign different priorities for the design goals at different levels. Designers can use the Archimedean formulation to consider many design goals requiring trade-offs at individual levels in a multilevel decision problem. In the Archimedean formulation, design goals in a priority set are assigned different weights to account for the differences in their relative importance [12]. The weights assigned are values between 0 and 1, summing to 1, with a higher value indicating a higher preference. Hence, the Archimedean formulation is used at individual levels of a multilevel decision problem. By combining the Preemptive and Archimedean formulations in the proposed framework, designers can account for many design goals requiring trade-offs at individual levels and relations across levels in PMMP systems using a c-cDSP. The c-cDSP is created and executed using the Decision Support In the Design of Engineering Systems (DSIDES) platform.

3.1.2. Robust design constructs: DCI and EMI

The DCI and EMI constructs help designers manage uncertainties by facilitating the identification of robust solutions that are relatively insensitive to uncertainties. Using the DCI construct [14], designers can account for design variable uncertainties arising from manufacturing processing and material microstructure variability. Using the EMI construct [15], designers can consider uncertainties in the models that interrelate processing with microstructure and microstructure with properties. The 'larger-is-better' and 'smaller-is-better' cases for EMI and DCI computations are depicted in Figures 4a and 4b, respectively.

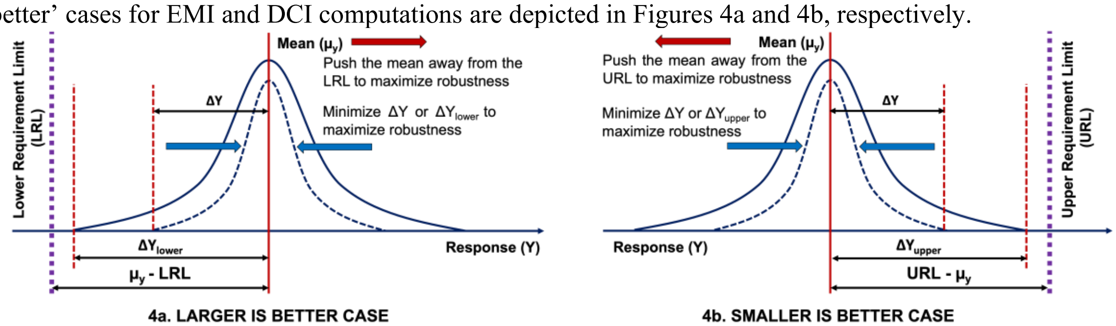

FIGURE 4: Uncertainty in responses with variability in design variables and models for the larger-is-better and smaller-is-better cases. The solid and the dashed bell curves represent different models for a response, indicating variability in the models.

Identifying solutions with values of DCI ≥ 1 and EMI ≥ 1 will ensure system robustness to uncertainties. The higher the DCI or EMI values, the higher the safety measure against failure due to uncertainties. A larger-is-better case is employed for maximization goals. The DCI and EMI values for the larger-is-better case are computed using Equations 1 and 4, respectively. For the l larger-is-better case depicted in Figure 4a, higher EMI and DCI values can be achieved by i) keeping the mean response (μ_y) as far away as possible from a lower requirement limit (LRL), thereby maximizing the numerator, and ii) minimizing the spread of the response - ΔY or $\Delta \mathrm{Y}_{\mathrm{lower}}$, thereby minimizing the denominator. A smaller-is-better case is employed for minimization goals. The DCI and EMI values for this case are computed using Equations 2 and 5, respectively. For the smaller-is-better case depicted in Figure 4b, higher EMI and DCI values can be achieved by i) keeping the mean response (μ_y) as far away as possible from an upper requirement limit (URL), thereby maximizing the numerator and ii) minimizing the spread of the response - ΔY or $\Delta \mathrm{Y}_{\mathrm{lower}}$, thereby minimizing the denominator.

For the larger-is-better case

$$DCI = \frac{\mu_y - LRL}{\Delta \mathrm{Y}} \tag{1}$$

For the smaller-is-better case

$$DCI = \frac{URL - \mu_y}{\Delta \mathrm{Y}} \tag{2}$$

where,

ΔY - response variation for small variations in design variables

μ_y– Mean responses

LRL – Lower requirement limit

URL – Upper requirement limit

The value of ΔY is computed as per Equation 3.

$$\Delta Y = \sum_{i=1}^{r} \left| \frac{\partial f}{\partial x_i} \right| * \Delta x_i \tag{3}$$

where,

i = 1, 2, 3, …, r (index of design variables)

Δx_i – variation or uncertainty in design variable x_i

$\frac{\partial f}{\partial x_i}$ – variation in the response f with respect to the design variable x_i

For the larger-is-better case

$$EMI = \frac{\mu_y - LRL}{\Delta Y_{lower}} \tag{4}$$

For the smaller-is-better case

$$EMI = \frac{URL - \mu_y}{\Delta Y_{upper}} \tag{5}$$

where,

μ_y – mean responses,

LRL – Lower requirement limit

$\Delta Y_{lower} = f_o(x) - Y_{min}$

$f_o(x)$ – mean response model

$Y_{min} = Min[\, f_j(x) - \Delta Y_j]$

j = 0, 1, 2, …, s (number of uncertainty bounds)

i = 1, 2, 3, …, r (index of design variables)

Δx_i – variation or uncertainty in design variable x_i

ΔY_j is the response variation for small variations in design variables for each uncertainty bound j and is computed as per Equation 6.

$$\Delta Y_j = \sum_{i=1}^{r} \left| \frac{\partial f_j}{\partial x_i} \right| * \Delta x_i \tag{6}$$

Given that the required data is available, an approach to generate the upper, mean, and lower bound models is presented in [34]. A discussion of this approach is beyond the scope of this paper. We do not employ the above approach in this paper. Instead, we assume the availability of the upper, mean, and lower bound models to demonstrate the facilitation of model uncertainty management using the framework.

3.1.3. iSOM visualization tool

iSOM [33] is a tool to visualize high-dimensional data using 2D plots. It is an unsupervised machine-learning algorithm, specifically an artificial neural network, and is a modified form of the conventional Self Organizing Maps (SOM) [35]. SOM, an artificial neural network developed by Kohonen [36], is an efficient algorithm for visualizing multidimensional numerical data [37]. The modification to conventional SOM results in the avoidance of self-intersections and makes the iSOM plots inherently interpretable. iSOM has distinct advantages, such as scalability and interpretability, making it suitable for exploring design space in real-world problems. Plots generated using iSOM are valuable for visualizing the underlying relationships between input design variables and output responses, as depicted in Figure 5 for the function $Z = X^2 + Y^2$.

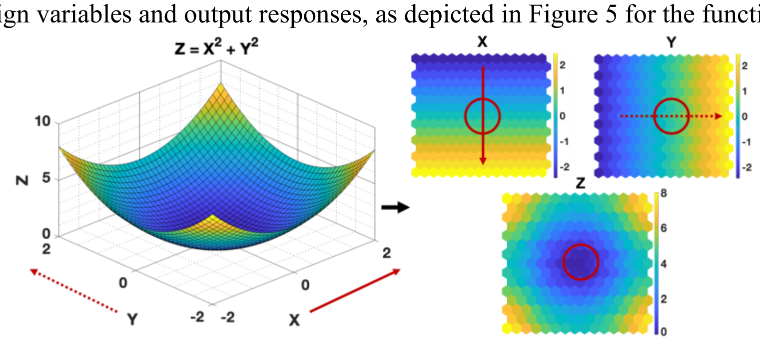

FIGURE 5: Example of visualization using iSOM for a function $Z = X^2 + Y^2$ (plot on the left) with input component plots X and Y and output component plot Z [38]

In Figure 5, the arrows in the X and Y component plots represent the increasing direction of the axes values. Correspondingly, the Z component plot captures the expected trend of a decrease followed by an increase in Z values with increasing X and Y values. Similarly, suppose designers are interested in the region the circle identifies in the Z component plot. They can determine the X and Y values that result in the chosen Z values. The circles in the X and Y component plots in Figure 5 identify these X and Y values. Using the iSOM plots, designers can carry out forward design space exploration to relate inputs to outputs and inverse design space exploration to relate outputs to inputs. It is worth noting that the shape of the function remains consistent in the Z component plot. A detailed discussion of selecting regions of interest using iSOM plots, regardless of the number of dimensions, is presented in [33]. The work by Sushil and co-authors [38] showcases the utility of the iSOM tool in visualizing i) high-dimensional design spaces and ii) the relations between inputs and outputs in multilevel systems. In recent literature, iSOM has been demonstrated as a potent visualization tool for effectively addressing multi-objective, multi-dimensional, and multi-criteria problem scenarios. More details can be found in [39-41]. In the proposed framework, we use iSOM to support the co-design exploration of the multilevel design spaces in PMMP systems by simultaneously visualizing the design spaces across individual levels using iSOM plots. The iSOM tool is available as a MATLAB code [33].

3.2. Decision support using the CoDE-MU framework

In this section, the structure and use of the CoDE-MU framework are discussed in detail. To demonstrate the concept, in the CoDE-MU framework presented, we only consider the interactions between two levels in the PMMP system – Design Levels 1 and 2. The CoDE-MU framework comprises four blocks named A, B, C, and D, as depicted in Figure 6. A detailed discussion of these blocks follows.

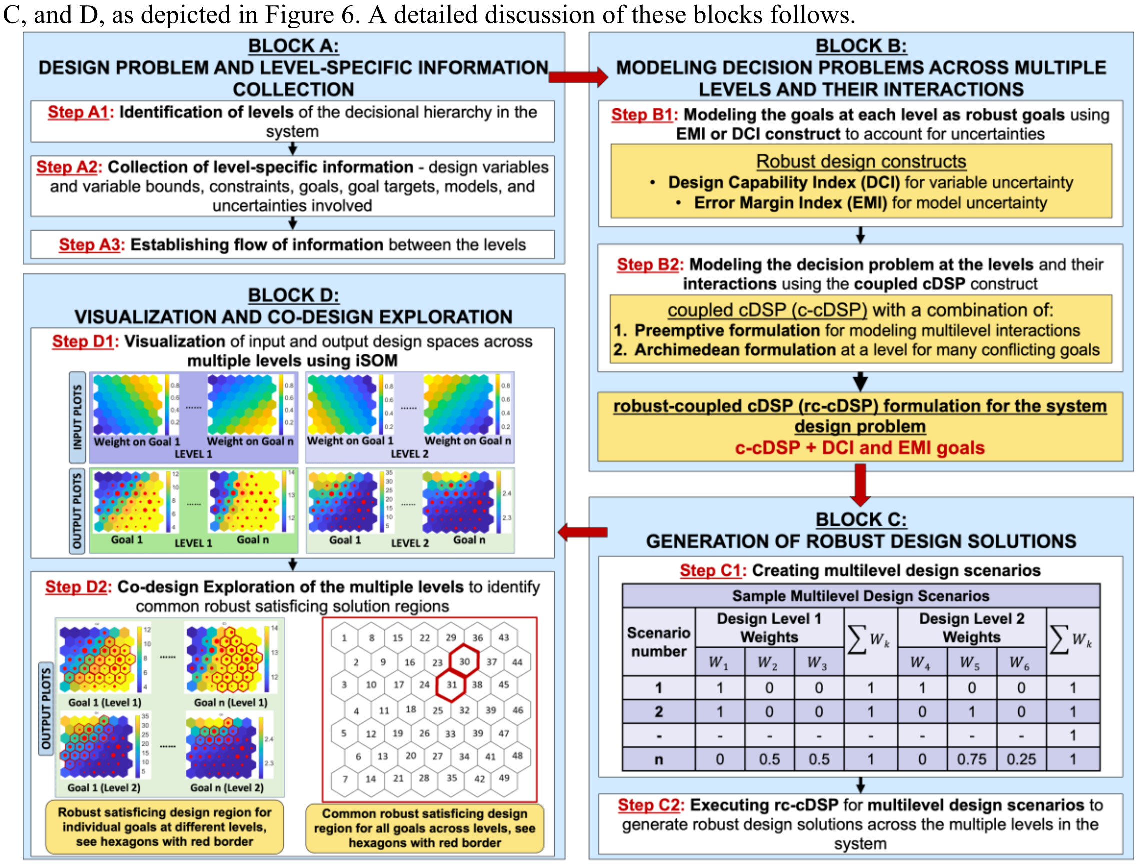

FIGURE 6: Decision support framework to facilitate multilevel robust co-design exploration of PMMP systems (Co-Design Exploration of Multilevel PMMP systems under Uncertainty: CoDE-MU)

Block A: Design problem and level-specific information collection

In Block A, information regarding the multilevel design problem and its levels are collected. Block A is executed in Steps A1 to A3, as discussed below.

<u>Step A1</u>: The levels of the decisional hierarchy in the multilevel PMMP system design problem are identified.

Step A2: Information specific to the decision problems at the individual levels is collected. The collected information includes i) design variables – their bounds and uncertainty estimates, ii) models employed and associated uncertainties, iii) design goals and goal targets, and iv) level-specific constraints.

Step A3: The flow of information connecting the individual levels is established by identifying shared design variables between levels. A copy of the shared design variables is used as the level-specific design variables at the lower level in the decision hierarchy. Additionally, consistency constraints are established at the lower level to ensure consistency of the shared design variable value at the lower level with the one determined at the upper level.

Block B: Modeling decision problems across individual levels and their interactions

In Block B, the decision problems at various levels in the PMMP system and their interactions are modeled as a single rc-cDSP using the information from Block A, as follows.

Step B1: Using the uncertainty information from Step A2, the design goals impacted by uncertainties at the individual levels are formulated as robust goals using the EMI and DCI constructs presented in Section 3.1.2. Goals affected by design variable uncertainties are formulated as DCI goals using Equations 1 or 2. Equations 1 and 2 are used when goals are maximization and minimization goals, respectively. Goals impacted by model uncertainties are formulated as EMI goals using Equations 4 or 5. Equations 4 and 5 are used when goals are maximization and minimization goals, respectively. A detailed description of EMI and DCI goal formulations for the HRR test problem is provided in Section 4. Step B1 is followed by Step B2, where the PMMP system design problem is modeled as an rc-cDSP.

Step B2: The individual-level decision problems and interactions across different levels in the PMMP system are modeled using the c-cDSP construct. In the c-cDSP, separate instances of the c-DSP construct are used to model decision problems at the individual levels. The keywords of the c-DSP construct – Given, Find, and Satisfy help capture the level-specific information. The interactions between the level-specific cDSPs in the c-cDSP are captured in the form of the flow of shared information, such as shared design variables, as determined in Step A3. In the c-cDSP, the goals impacted by uncertainties are formulated as DCI and EMI goals, as discussed in Step B1. The c-cDSP with EMI and DCI goals is referred to as the rc-cDSP. The deviation function of the rc-cDSP is modeled using a combination of Preemptive and Archimedean formulations. Decisions in PMMP systems are made hierarchically across levels. Hence, the Preemptive formulation is employed, where the design goals at Design Levels 1 and 2 are assigned different priority levels. Design Level 1 decisions are given higher priority as these are made first, followed by Design Level 2 decisions at a lower priority. The difference in preferences among the many design goals at individual levels of a multilevel decision problem is modeled using the Archimedean formulation, where different weights are assigned to the various goals. The weights assigned are values between 0 and 1 that sum up to 1, with higher values indicating higher preference. Combining the Preemptive and Archimedean formulations in the rc-cDSP allows designers to consider many design goals requiring trade-offs at individual levels and relations across levels of a multilevel decision problem, using a coupled decision problem formulation. A detailed description of the rc-cDSP for the HRR test problem is provided in Section 4. The rc-cDSP is created using the DSIDES platform.

Block C: Generation of robust design solutions

In Block C, the rc-cDSP formulation is executed for different multilevel design scenarios using the DSIDES platform to generate robust design spaces across multiple levels. Block C is implemented in two steps.

Step C1: The multilevel design scenarios to execute the rc-cDSP are created. The multilevel design scenarios depicted in Step C1, Block C of Figure 6, represent situations with different preferences for the design goals across Design Levels 1 and 2. These multilevel design scenarios are created by combining individual-level design scenarios at Design Levels 1 and 2 in all possible combinations. Individual-level design scenarios are created using Latin hypercube sampling. In each individual-level design scenario, different weights are assigned to the design goals at the level. The weights indicate the difference in preferences amongst the goals. The weights assigned are values between 0 and 1 that add up to 1, with higher values indicating higher preference. If there are ‘n’ distinct design scenarios at an individual level in a multilevel PMMP system with ‘m’ levels, there exist n^m distinct multilevel design scenarios. In this paper, n^2 multilevel design scenarios are considered for the two-level PMMP system.

Step C2: The rc-cDSP formulation for the PMMP system is exercised for the n^2 multilevel design scenarios to generate design solutions, including robust solutions, across the levels.

Block D: Visualization and co-design exploration

In Block D, the simultaneous visualization of individual-level solution spaces is carried out using iSOM. This is followed by the co-design exploration of individual-level solution spaces to identify common robust satisficing solutions across multiple levels. Block D is executed in two steps, as detailed below.

Step D1: The iSOM algorithm is trained for the weight combinations corresponding to different multilevel design scenarios and goal values generated for these scenarios. The trained iSOM algorithm produces separate 2D iSOM plots for each input weight and output goal across multiple levels. The simultaneous visualization of the individual-level solutions spaces across various levels is realized by combining iSOM with the rc-cDSP. The iSOM plots for the output goals help designers visualize the relations between goals across multiple levels.

Step D2: The solution spaces visualized using iSOM plots are explored to determine satisficing solution regions for the individual goals by setting satisficing limits for each goal. The hexagonal grid points in an iSOM plot whose values meet the set satisficing limit constitute the satisficing solution region for a given goal. For example, in Step D2, Block D of Figure 6, the iSOM grid points with red borders identify the satisficing solution regions for the individual goals. Only the grid points with multilevel design scenarios mapped against them, indicated by the dots on the iSOM grid points, are considered. A larger size of the dot on an iSOM grid point suggests a larger number of multilevel design scenarios being mapped to that specific iSOM grid point. The designers seek to identify common satisficing solution regions for all the goals across the levels by carrying out co-design exploration. Co-design exploration is carried out using a systematic approach described as follows.

Systematic co-design exploration: Systematic co-design exploration takes place in 3 steps.

Step 1: Determining if satisficing goal limit relaxations are required.

The designer asks, "Does a common satisficing solution region exist for all the goals across the levels?”

- If “No,” the designer proceeds to Step 2.
- If “Yes,” co-design exploration is complete, and common satisficing solutions for all goals across levels are identified.

Step 2: Identifying a goal to be excluded from satisficing limit relaxation.

The designer identifies a goal across the different levels whose satisficing limits cannot be relaxed due to its critical nature. The following goals are candidates to be excluded from satisficing limit relaxation: i) goals formulated as DCIs or EMIs with low satisficing limit values, typically less than 1.5, and ii) other goals deemed critical by designers. All the remaining goals are collectively called ‘non-excluded’ goals.

Step 3: Relaxation of satisficing limits for non-excluded goals.

The designer begins by grouping all non-excluded goals into two sets: i) Set 1 - All non-excluded goals formulated as DCIs or EMIs with satisficing limit values greater than 1.5, and ii) Set 2 - All remaining non-excluded goals. The relaxation of satisficing limits of non-excluded goals starts with the goals in Set 1, followed by the goals in Set 2.

Step 3a: Relaxation of satisficing limits for Set 1 goals.

- The designer picks the goal in Set 1 with the highest satisficing limit defined in terms of DCI or EMI value.
- For the chosen goal, the designer checks for any common iSOM grid points between the satisficing solution regions of the excluded and chosen goals.
    - If any common iSOM grid points exist, the satisficing limits of the chosen goal are not relaxed. The designer then picks the goal in Set 1 with the next highest DCI or EMI satisficing limit value and repeats the check.
    - If no common iSOM grid points are identified, the designer relaxes the satisficing limit by the least possible amount till common iSOM grid points are identified. The relaxed DCI or EMI satisficing limits can be as low as 1.5.
    - The above step is repeated till all goals in Set 1 are considered.

Step 3b: Relaxation of satisficing limits for Set 2 goals.

- Based on the designer’s judgment, a goal in Set 2 with a greater scope for satisficing limits relaxation is chosen.
- For the chosen goal, the designer repeats the procedure to check for common iSOM grid points described in Step 3a until all goals in Set 2 are considered.

At the end of Step 3b, designers identify a common satisficing region for all the goals across different levels, as depicted by the plot labeled ‘common robust satisficing design region for all goals across levels’ in Step D2 of Figure 6. Based on the common region identified, the designer then determines the design scenarios mapped to the common region and the corresponding design variable and goal values. The designer can also use the input and output iSOM component plots to understand the effect of varying the weights and changing variable values on the goals across multiple levels and other performance indicators in PMMP systems. In the next section, we demonstrate the CoDE-MU framework's efficacy in supporting the design of multilevel PMMP systems using an industry-inspired steel manufacturing process chain problem.

4. THE HOT ROD ROLLING (HRR) PMMP SYSTEM DESIGN PROBLEM

The CoDE-MU framework's efficacy is tested using the industry-inspired Hot Rod Rolling (HRR) problem. In this problem, we look at the co-design of the HRR PMMP system composed of the hot rolled rod product, C-Mn steel material, and the cooling manufacturing process. HRR of steel is a complex manufacturing process chain used to produce hot-rolled steel rods as products. HRR comprises a series of manufacturing processes executed sequentially, as depicted in Figure 7, starting with the 'reheating process,' where the primary input steel in the form of billets is reheated. The reheated steel billets are then plastically deformed to steel rods in the 'hot rolling process' by passing the material through several rollers in rolling mills. Further, the 'cooling process' is carried out where rolled products are cooled in a run-out table to produce steel rods as products.

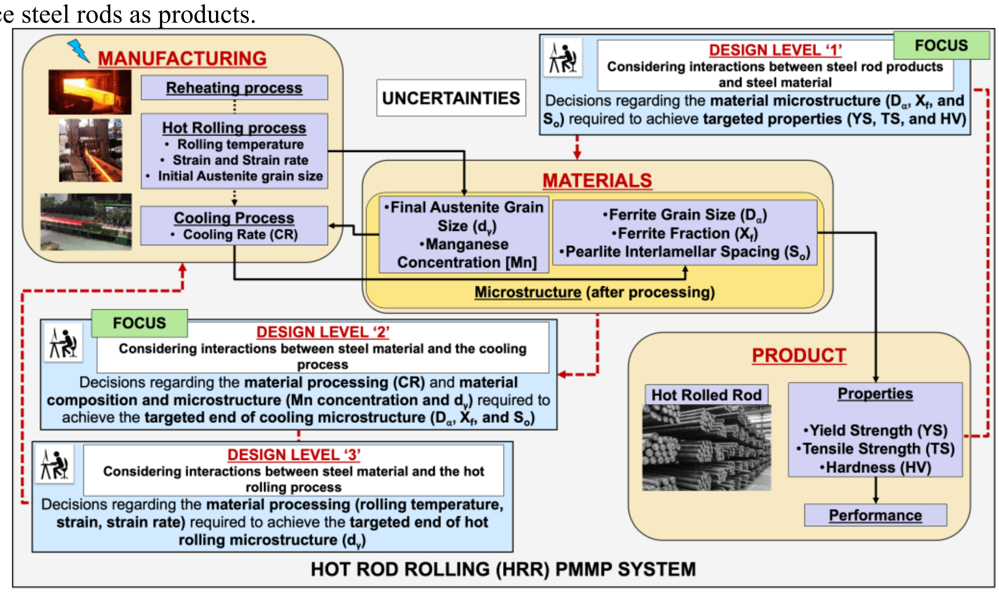

FIGURE 7: Multilevel decision-making and their interrelations in the HRR PMMP system

The above thermo-mechanical processing during manufacturing causes microstructural evolution and macrostructural changes in the material, resulting in hot-rolled steel rods with specific microstructural characteristics and corresponding mechanical properties. The performance requirements of the steel rods are identified in terms of the target mechanical properties of the rods. Realizing hot rolled rods with targeted performance requires the collective consideration of i) manufacturing processing, ii) material microstructure and composition, and iii) product properties. In this paper, to demonstrate the efficacy of the CoDE-MU framework, we bound the HRR PMMP system design problem to consider only the cooling process in the HRR process chain. The design of the HRR PMMP system using the CoDE-MU framework is discussed below.

Block A: The HRR PMMP system and design level-specific information collection.

The design of the HRR PMMP system starts at Step A1 in Block A of the CoDE-MU framework.

<u>Step A1</u>: The levels of decisions in the HRR PMMP system are identified. The design of the HRR PMMP system involves decisions at three levels – Design Levels 1, 2, and 3, as depicted in Figure 7. Design Level 1 involves decisions regarding materials that affect product properties and performance. Design Levels 2 and 3 involve decisions regarding the cooling and rolling manufacturing processing, respectively, that affect the material. To demonstrate the efficacy of the CoDE-MU framework, we focus on Design Levels 1 and 2 and their interactions only. This aspect is clarified in Figure 7 using the block labeled 'FOCUS' beside Design Levels 1 and 2.

<u>Step A2</u>: Information specific to Design Levels 1 and 2 is collected. At Design Level 1, decisions are made regarding i) the steel microstructure design variables identified by the Ferrite grain size (D_α), Ferrite fraction (X_f), and Pearlite interlamellar spacing (S_o) and ii) the steel composition design variable identified by Manganese concentration [Mn] to achieve required mechanical properties for the steel rods. The

mechanical property requirements are to achieve targeted Yield strength (YS), Tensile strength (TS), and Hardness (HV) values of 330MPa, 750MPa, and 170, respectively. The corresponding minimum acceptable values of 220MPa, 450MPa, and 130 define the lower requirement limits. The YS, TS, and HV property requirements have different behaviors, and simultaneously realizing these properties requires compromises or trade-offs. In Appendix A1, the models that relate the mechanical properties to the steel microstructure and composition design variables at Design Level 1 are listed. The concentration of other elements that determine the steel composition (Fe, C, Si, N, P, and Cu) is assumed to be fixed. The Design Level 1 specific information is listed in the Given Section of Table 1.

At Design Level 2, decisions are made regarding i) the cooling process design variable - Cooling Rate (CR), ii) the input steel microstructure design variable - Austenite grain size (d_γ), and iii) the input steel composition design variable - [Mn] to achieve the required end of cooling steel microstructure. The end of cooling steel microstructure requirements are to achieve the targeted D_α, S_o, and X_f values of 5µm, 0.15µm, and 1.0, respectively. The acceptable values D_α = 20µm, S_o = 0.2µm, and X_f = 0.6 define the upper requirement limits for D_α and S_o and the lower requirement limit for X_f. The models that relate the steel microstructure at the end of cooling to the cooling processing and input material microstructure and composition design variables at Design Level 2 are provided in Appendix A2. The Design Level 2 specific information is provided in the Given Section of Table 1.

The decisions at Design Levels 1 and 2 are subject to uncertainties associated with design variables. We consider uncertainty in the model that relates YS to the steel microstructure at Design Level 1 using three different YS models. Based on the values predicted for YS, we assume the model by Gladman and co-authors [42] as the mean model - $f_o(x)$ or YS_{mean}, the model by Hodgson and Gibbs [43] as the upper bound - $f_1(x)$ or YS_{upper}, and the model by Kuziak and co-authors [44] as the lower bound model - $f_2(x)$ or YS_{lower}. These models are presented in Appendix A1. We assume no model uncertainties for the remaining requirements across Design Levels 1 and 2. The uncertainties associated with the design variables at Design Levels 1 and 2 are listed in the Given Section of Table 1.

<u>Step A3</u>: The design level-specific information from Step A3 is employed to identify the relationship between the design levels regarding shared design variables. [Mn] is the shared design variable between Design Levels 1 and 2. Hence, a copy of this variable, [Mn_{copy}], is used at Design Level 2 as its level-specific variables. Additionally, a consistency constraint is imposed at Design Level 2 to ensure that the value of the [Mn] design variable at both levels remains the same. These details are provided in the Given and Satisfy Sections of Table 1.

Block B: Modeling decision problems across multiple levels in the HRR PMMP system and their interactions

Using the information from Block A, decisions at Design Levels 1 and 2 and their interactions are modeled in steps B1 and B2.

<u>Step B1</u>: Based on the uncertainty information from Step A2, the goals at Design Levels 1 and 2 are formulated as robust goals using the EMI and DCI constructs. At Design Level 1, the YS requirement is formulated as an EMI goal to account for uncertainties in the YS model. The formulation of the EMI YS goal using Equation 3 is discussed below.

$$EMI\ YS = \frac{\mu_y - LRL}{\Delta Y_{lower}}$$

where,

LRL= 220MPa

μ_y is the YS_{mean} or $f_o(x)$ model in Table A1, Appendix A

$\Delta Y_{lower} = f_o(x) - Y_{min}$

$Y_{min} = Min[\, f_j(x) - \Delta Y_j]$, where j= 0, 1, and 2 corresponding to the mean, upper and lower bound models for YS, respectively, in Table A1, Appendix A

$\Delta Y_j = \sum_{i=1}^{4} |\frac{\partial f_j}{\partial x_i}| * \Delta x_i$, where i= 1, 2, 3, and 4 corresponding to design variables X_1 to X_4 at Design Level 1, for every j= 0, 1, and 2.

The TS and HV goals at Design Level 1 are formulated as DCI goals to account for design variable uncertainties that arise from the variability in steel microstructure - D_α, S_o, and X_f and steel composition [Mn]. The DCI TS goal formulation using Equation 1 is presented below as an example.

$$DCI = \frac{\mu_y - LRL}{\Delta Y}$$

where,

LRL= 450MPa

μ_y or f is the TS model in Table A1, Appendix A

$\Delta Y = \sum_{i=1}^{4} \left|\frac{\partial f}{\partial x_i}\right| * \Delta x_i$, where i= 1, 2, 3, and 4 corresponding to design variables X_1 to X_4 at Design Level 1

The D_α, S_o, and X_f goals at Design Level 2 are formulated as DCI goals to facilitate the consideration of design variable uncertainties that arise from the variability in cooling processing parameter – CR, steel microstructure - d_γ, and steel composition - [Mn_{copy}]. The EMI and DCI goal formulations at Design Levels 1 and 2 are maximization goals to achieve higher EMI and DCI values, thereby ensuring greater robustness to uncertainties. The EMI YS, DCI TS, and DCI HV goal targets are set as 3, 8, and 8, respectively. The goal targets for DCI D_α, DCI S_o, and DCI X_f are set as 3, 10, and 10, respectively.

Step B2: Using the information from Block A, the decisions at Design Levels 1 and 2 and interactions are modeled using the c-cDSP construct. In the c-cDSP, a copy of the [Mn] shared design variable and a consistency constraint are employed at Design Level 2 to account for the interactions, as listed in the Satisfy Section in Table 1. The DCI and EMI goal formulations from Step B1 are used as goals for the c-cDSP. The DCI and EMI goals and the c-cDSP together form the rc-cDSP for the HRR PMMP system, as detailed in Table 1. Further design requirements pertaining to cost or other production considerations may be added as goals at the appropriate design level in the rc-cDSP. Additionally, constraints, as listed in the Satisfy Section in Table 1, are established to i) ensure DCI and EMI goal values greater than one and guarantee robust solutions and ii) to account for any limitations associated with the manufacturing processing. The deviation function of the rc-cDSP is modeled using a combination of Preemptive and Archimedean formulations. The decisions in the HRR PMMP system are made hierarchically, with decisions at Design Level 1 being made before the decisions at Design Level 2. The Preemptive formulation is employed to help account for the hierarchical relation between Design Levels 1 and 2. The difference in preferences among the many design goals at the individual levels - Design Levels 1 and 2, is modeled using the Archimedean formulation, as given in the Minimize Section in Table 1. By combining the Preemptive and Archimedean formulations in the rc-cDSP, designers can consider many goals at Design Levels 1 and 2 and relations between Design Levels 1 and 2 in a coupled decision problem formulation.

TABLE 1: Robust coupled cDSP (rc-cDSP) for the HRR PMMP system considering interactions between Design Levels 1 and 2

GIVEN
a. HRR PMMP system information Constants: i. Elemental composition of C-Mn steel: [Cu]= 0.08%; [P]= 0.019%; [C]= 0.18%; [N]= 0.007%; [Si]= 0.36% ii. Average Austenite to Ferrite transition temperature, T_{mf} = 700^{0}C iii. Pearlite colony size, p= 6μm, iv. Carbide thickness, t_{carb}= 0.025μm v. Residual strain at the end of rolling, ε_r = 0 (assumed)
b. Design variables (x_i), their bound, and uncertainties at Design Level 1 i. $0.1 \leq x_1 (X_f) \leq 1.0$ ii. $5 \leq x_2 (D_\alpha) \leq 25$ (μm) iii. $0.15 \leq x_3 (S_0) \leq 0.25$ (μm) iv. $0.7 \leq x_4$ ([Mn]) ≤ 1.5 (%) ***(shared)*** • Uncertainty: D_α= ± 3μm; X_f= ± 0.1; S_o= ± 0.01μm; [Mn]= ± 0.1% Design variables (x_i), their bounds, and uncertainties at Design Level 2 i. $30 \leq x_5 (d_\gamma) \leq 100$ (μm) ii. $0.1833 \leq x_6$ (CR) ≤ 1.66 (ºC/s) iii. $0.7 \leq x_7$ ([Mn_{copy}]) ≤ 1.5 (%) ***(shared)*** • Uncertainty: d_γ= ± 10μm; CR= ± 0.166ºC/s; [Mn_{copy}]= ± 0.1%
c. End requirements at Design Level 1 in terms of steel rod mechanical properties i. Achieve targeted YS [MPa] ii. Achieve targeted TS [MPa] iii. Achieve targeted HV Corresponding requirement on the rc-cDSP goals (G_k) at Design Level 1 (k= 1,2,3)

i. Goal G_1: Maximize EMI YS ii. Goal G_2: Maximize DCI TS iii. Goal G_3: Maximize DCI HV Goal Targets: $G_{1,target} = 3$; $G_{2,target} = 8$; $G_{3,target} = 8$ End requirements at Design Level 2 in terms of steel microstructural characteristics i. Achieve targeted D_α ii. Achieve targeted S_0 iii. Achieve targeted X_f Corresponding requirement on the rc-cDSP goals (G_k) at Design Level 2 (k= 4,5,6) i. Goal G_4: Maximize DCI D_α ii. Goal G_5: Maximize DCI S_0 iii. Goal G_6: Maximize DCI X_f Goal Targets: $G_{4,target} = 3$; $G_{5,target} = 10$; $G_{6,target} = 10$ • The models for the end requirements at Design Levels 1 and 2 are provided in Appendix A1 and A2, respectively. • Uncertainty associated with the YS model is represented by the YS_{mean}, YS_{upper}, and YS_{lower} models listed in Appendix A1.
d. Requirement limits at Design Level 1: Lower Requirement Limit (LRL) for YS_{mean}= 220MPa; LRL for TS= 450MPa; LRL for HV= 130 Requirement limits at Design Level 2: Upper Requirement Limit (URL) for D_α= 25μm; URL for S_0= 0.25μm; LRL for X_f= 0.5
FIND values of
a. Design variables: X_i, where i= 1,2,3,4,5,6,7
b. Deviation variables: d_k^+ and d_k^-, where k= 1,2,3,4,5,6
SATISFY
a. Design Level 1 constraints ii. EMI YS ≥ 1 iii. DCI TS ≥ 1 iv. DCI HV ≥ 1 Design Level 2 constraints i. $d_\gamma \leq 100$ ii. $d_\gamma \geq 30$ iii. CR ≤1.66 iv. CR ≥0.1833 v. Mn_{copy}= Mn ***(consistency constraint for shared design variable)*** vi. DCI D_α ≥ 1 vii. DCI S_0 ≥ 1 viii. DCI X_f ≥ 1
b. Variable bounds at Design Level 1 i. $0.1 \leq X_f \leq 1.0$ ii. $5 \leq D_\alpha \leq 25$ iii. $0.15 \leq S_0 \leq 0.25$ iv. $0.7 \leq [Mn] \leq 1.5$ Variable bounds at Design Level 2 i. $30 \leq d_\gamma \leq 100$ ii. $0.1833 \leq CR \leq 1.66$ iii. $0.7 \leq [Mn_{copy}] \leq 1.5$ Deviation variable bounds $d_k^+, d_k^- >= 0$ and $d_k^+ * d_k^- = 0$
MINIMIZE
Preemptive formulation at two levels. The deviation function (Z) needs to be minimized. Min Z= (f_1, f_2) Priority 1: Design Level 1 (Archimedean Formulation) $f_1 = \boldsymbol{\Sigma}\, W_k (d_k^+ + d_k^-)$,

where, W_k= weights assigned to the deviations of the individual goals from the target values, $\boldsymbol{\Sigma}$ W_k= 1, and k= 1, 2, 3.

Priority 2: Design Level 2 (Archimedean Formulation)

$$f_2 = \boldsymbol{\Sigma}\, W_k\,(d_k^{+} + d_k^{-}),$$

where, W_k= weights assigned to the deviations of the individual goals from the target values, $\boldsymbol{\Sigma}$ W_k= 1 and k= 4, 5, 6

Block C: Generation of robust design solutions across Design Levels 1 and 2

The rc-cDSP is executed for various multilevel design scenarios to generate robust design solutions across Design Levels 1 and 2.

Step C1: Multilevel design scenarios are created by considering all combinations of individual-level design scenarios at Design Levels 1 and 2. Individual-level design scenarios are created by assigning different combinations of weights to the goals at the level using a Latin hypercube sampling (LHS) design. Using the LHS design helps cover the design space effectively. 13 design scenarios are considered at the individual levels, leading to 169 multilevel design scenarios across the two design levels. Some sample multilevel design scenarios are listed in Table 2.

TABLE 2: Sample multilevel design scenarios

Scenario #	Design Level 1 weights ($W_{k=1,2,3}$)				Design Level 2 weights ($W_{k=4,5,6}$)			
	W_1	W_2	W_3	$\sum_k W_k$	W_4	W_5	W_6	$\sum_k W_k$
1	0.33	0.13	0.54	1	0.33	0.13	0.54	1
2	0.33	0.13	0.54	1	0.35	0.42	0.23	1
-	-	-	-	-	-	-	-	-
55	0.16	0.42	0.42	1	0.06	0.06	0.88	1
-	-	-	-	-	-	-	-	-
169	0.33	0.18	0.49	1	0.33	0.18	0.49	1

Step C2: The HRR PMMP system rc-cDSP is executed for the multilevel design scenarios to generate robust design solutions for the goals across Design Levels 1 and 2.

Block D*:* Visualization and co-design exploration of the solution spaces

In Block D, the visualization and co-design exploration of the robust solution spaces across Design Levels 1 and 2 is carried out in Steps D1 and D2, respectively.

Step D1: The weight combinations corresponding to different multilevel design scenarios and goal values generated for these scenarios at Design Levels 1 and 2 are used to train the iSOM algorithm. The trained iSOM helps visualize the solution spaces across the levels simultaneously by generating six iSOM plots for the six goals across Design Levels 1 and 2, as shown in Figure 8.

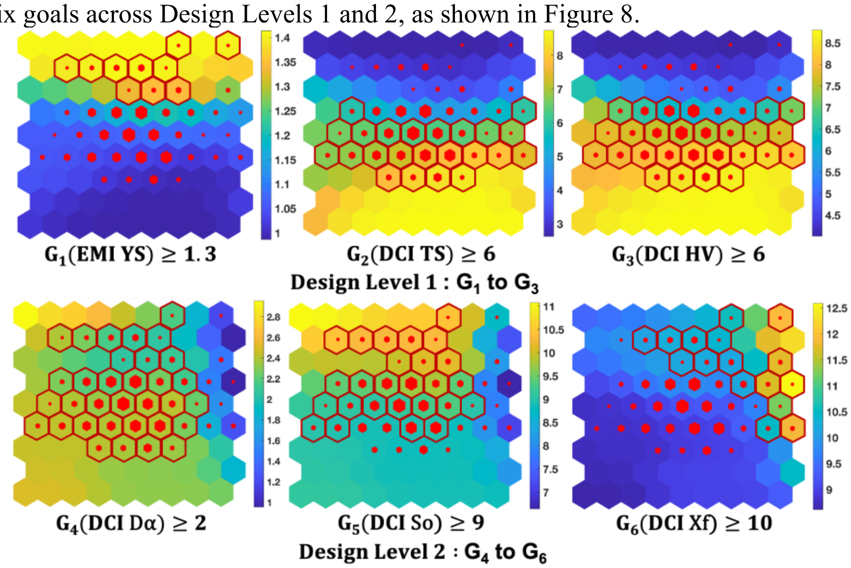

FIGURE 8: Initial iSOM plots for goals at Design Levels 1 and 2, with yellow and dark blue regions representing relatively high and low robustness regions, respectively. The hexagonal iSOM grid points highlighted in red indicate satisficing solutions regions for goals. The red dots indicate design scenarios being mapped to the iSOM grid points.

Step D2: The iSOM plots for the goals are used to conduct co-design exploration of Design Levels 1 and 2 by simultaneously exploring the solution spaces. Co-design exploration of the levels helps identify common robust satisficing solutions for the goals across the two levels.

The co-design exploration of Design Levels 1 and 2 begins by establishing the satisficing limits for all the goals to identify robust satisficing solution regions on the iSOM plots for each goal. The designer focuses on ensuring greater safety against uncertainties by choosing regions with higher EMI or DCI values. Hence, the satisficing limits for the goals at Design Levels 1 and 2 are initially set to the higher end of the achievable EMI or DCI values, as follows.

At Design Level 1

i. EMI YS, $G_1 \geq 1.3$

ii. DCI TS, $G_2 \geq 6$

iii. DCI HV, $G_3 \geq 6$

At Design Level 2

i. DCI D_α, $G_4 \geq 2$

ii. DCI S_o, $G_5 \geq 9$

iii. DCI X_f, $G_6 \geq 10$

For the above satisficing goal limits, iSOM grid points highlighted with a red border in Figure 8 indicate the initial satisficing solution regions.

Systematic co-design exploration

Step 1: With the satisficing limits set to the above values, the designer identifies no common region in terms of iSOM grid points for all six goals across Design Levels 1 and 2. The designer, therefore, proceeds to Step 2.

Step 2: Since all the goals are formulated as EMIs or DCIs, the designer picks the goal with the lowest satisficing limit as the goal to be excluded from satisficing limit relaxation. Hence, G_1, with a satisficing limit of less than 1.5, is picked as the goal to be excluded from the satisficing limit relaxation. G_2 to G_6 constitute the non-excluded goals.

Step 3: The designer groups all non-excluded goals (G_2 to G_6) into Set 1 as they are all formulated as DCIs or EMIs.

Step 3a: The designer picks G_6 with the largest satisficing limit value. Since common grid points with the excluded goal G_1 are identified, as depicted by the iSOM grid points highlighted in black for G_1 and G_6 in Figure 9, the satisficing limit of G_6 is not relaxed. The designer then picks the goals with the next highest satisficing limit, G_5. The designer checks for common grid points and decides not to relax the satisficing limit for G_5 as common grid points exist. The designer then considers G_3. Since G_3 has no common iSOM grid points with the excluded goal G_1, G_3's satisficing limit is relaxed to 5. This results in the iSOM grid points highlighted in black in Figure 9 becoming common for G_3 and G_1. The above step is repeated for G_2, resulting in its satisficing limit being relaxed to 3.5. Finally, the designer considers G_4 with the smallest satisficing limit in Set 1. Since G_4 has common iSOM grid points with the excluded goal G_1, G_4's satisficing limit is not relaxed.

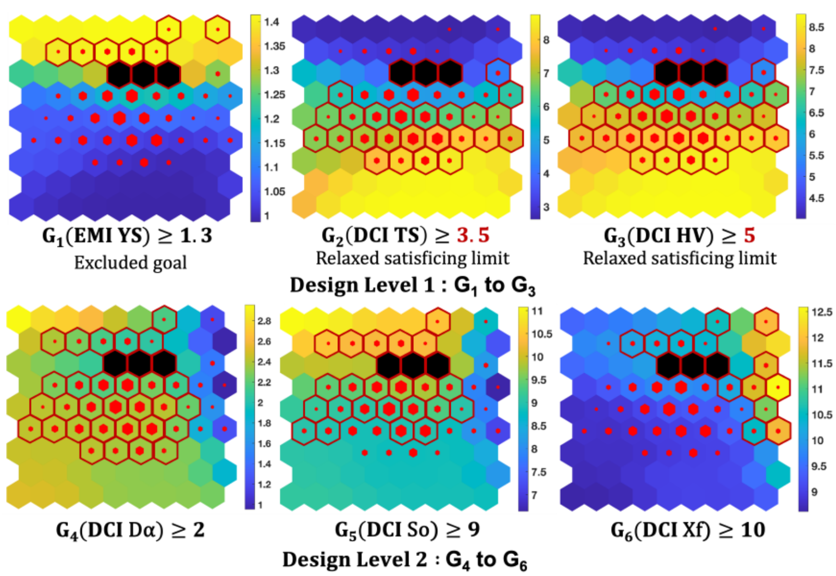

FIGURE 9: iSOM plots for all goals across Design Levels 1 and 2 after systematically updating the satisficing goal limits. The iSOM grid points highlighted in red indicate the satisficing solutions regions for the goals. The black iSOM grid points indicate the common satisficing solution region for all Design Levels 1 and 2 goals.

With the updated satisficing limits, three iSOM grid points are determined to be the common satisficing region for all the goals, as depicted by the black iSOM grid points in Figure 9. These grid points have six design scenarios mapped against them, resulting in six common robust satisficing design solutions across Design Levels 1 and 2 of the HRR PMMP system. Hence, using the combination of the rc-cDSP and iSOM in the CoDE-MU framework, designers can simultaneously explore the solution spaces across Design Levels 1 and 2 to identify common robust satisficing design solutions. The CoDE-MU framework thereby facilitates the robust co-design of the HRR PMMP system. The six design scenarios and the corresponding goal values at Design Levels 1 and 2 are listed in Table 3.

TABLE 3: Common solutions identified after co-design exploration of Design Levels 1 and 2 in the HRR PMMP system

Design Scenario #	Robust goal values					
	Design Level 1			Design Level 2		
	EMI YS	DCI TS	DCI HV	DCI D_α	DCI S_0	DCI X_f
40	1.45	3.25	4.62	2.00	10.40	10.21
44	1.45	3.25	4.62	1.67	9.75	10.84
49	1.45	3.25	4.62	2.00	10.40	10.21
50	1.45	3.25	4.62	1.67	9.75	10.84
52	1.45	3.25	4.62	2.00	10.40	10.21
144	1.45	3.25	4.62	2.00	10.40	10.21

On analyzing the EMI and DCI values in Table 3, all solutions identified are robust with EMI and DCI values greater than 1. The design variables values, steel rod properties, and steel microstructure corresponding to the six common robust satisficing design solutions are listed in Table 4.

TABLE 4: Design variables, properties, and microstructure corresponding to the common robust satisficing solutions identified after co-design exploration of Design Levels 1 and 2 in the HRR PMMP system

Design Scenario #	Design Variables							Properties and Microstructure					
	Design Level 1				Design Level 2			Design Level 1			Design Level 2		
	X_f	D_α	S_0	Mn	d_γ	CR	Mn_{copy}	YS_{mean}	TS	HV	D_α	S_0	X_f
		µm	µm	%	µm	°C/s	%	MPa	MPa		µm	µm	
40	0.52	8.50	0.15	1.50	42.50	1.16	1.50	341.53	617.03	151.23	18.87	0.11	0.67
44	0.52	8.50	0.15	1.50	42.50	0.98	1.50	341.53	617.03	151.23	19.51	0.12	0.68
49	0.52	8.50	0.15	1.50	42.50	1.16	1.50	341.53	617.03	151.23	18.87	0.11	0.67
50	0.52	8.50	0.15	1.50	42.50	0.98	1.50	341.53	617.03	151.23	19.51	0.12	0.68
52	0.52	8.50	0.15	1.50	42.50	1.16	1.50	341.53	617.03	151.23	18.87	0.11	0.67
144	0.52	8.50	0.15	1.50	42.50	1.16	1.50	341.53	617.03	151.23	18.87	0.11	0.67

Upon analyzing the mechanical properties of steel rods listed in Table 4, a mean YS of 341.53MPa, TS of 617.03MPa, and HV of 151.23 are achieved by ensuring a steel microstructure with moderate to high X_f (0.52), low D_α (8.5µm), low S_0 (0.15µm), and steel composition with [Mn] of 1.5%. At Design Level 2, the cooling process parameter (CR), input steel microstructure (d_γ), and composition ([Mn]) variable values identified help achieve targeted X_f, D_α, and S_0 values, given the cooling process constraints and uncertainties involved. This results in D_α values between 18.9 and 19.5µm, S_0 values between 0.11 and 0.12µm, and X_f values between 0.67 and 0.68, as listed in Table 4. Correspondingly, the cooling rate during the cooling process is identified to be between 0.98 and 1.16°C/s, and the input steel microstructure, d_γ of 42.5µm. Based on the CR value range, it is evident that higher cooling rates are necessary to realize the required steel microstructure and steel rod properties. Therefore, designers can assess the impact of process variables on the product and materials using the CoDE-MU framework.

From the iSOM plots in Figure 9, the relations among the goals at the individual levels can also be ascertained. For example, at Design Level 1, a focus on achieving high EMI YS, depicted by the yellow regions on the iSOM plot for G_1, will result in lower DCI TS and DCI HV values, shown by the blue regions on the G_2 and G_3 iSOM plots. Similarly, at Design Level 2, a focus on maximizing DCI X_f, depicted by the yellow regions in the iSOM plot for G_6, will result in lower DCI S_o and DCI D_α values, shown by the blue regions on the G_4 and G_5 iSOM plots. Moreover, the relations among the goals across levels can also be established based on the iSOM plots. For example, a focus on achieving high DCI S_o and DCI D_α values at

Design Level 2, depicted by the yellow regions on the G_4 and G_5 iSOM plots, will result in high EMI YS value, represented by the yellow regions in the G_1 iSOM plot, and low DCI TS and DCI HV values, represented by the blue regions in the G_2 and G_3 iSOM plots, at Design Level 1. Therefore, the CoDE-MU framework also supports designers in understanding the relations within and between levels during the design of the HRR PMMP system.

5. CLOSING REMARKS

Realizing products that simultaneously meet many performance requirements with different behaviors requires careful consideration of the relations among the product, materials, and manufacturing processes across multiple decision levels in PMMP systems. Failure to account for the relations among individual levels will result in design conflicts that will adversely impact the realization of targeted product performance. Uncertainties arising from the variability associated with processing and microstructure and uncertainties in the models employed will also adversely affect product performance. Hence, it is vital to consider the relations among individual levels and manage the design conflicts and uncertainties during PMMP systems design. This necessitates the support for co-design exploration of individual design levels to identify ranged sets of common robust satisficing solutions across the levels.

In this paper, we present a decision support framework that facilitates the co-design exploration of multiple levels of the PMMP systems under uncertainty, namely CoDE-MU. In the CoDE-MU framework, the c-cDSP construct is combined with EMI and DCI robust design constructs and machine-learning-based iSOM visualization to facilitate multilevel robust co-design exploration. Using the framework, designers can i) model decision problems across individual levels and their interactions using a coupled decision problem formulation, ii) visualize and simultaneously explore the design spaces across multiple levels, iii) manage the impact of uncertainties, and iv) identify important processing and microstructure variables that influence the product performance. The framework enhances the ability of designers to account for the interactions among the products, materials, and manufacturing processes and, at the same time, manage the inherent uncertainties in PMMP systems. This is achieved by employing the rc-cDSP, where the c-cDSP construct is used with the EMI and DCI robust design constructs. In the rc-cDSP, a combination of the Preemptive and Archimedean formulations is employed to help account for i) the hierarchical relationships among the individual levels and ii) the many design goals requiring trade-offs at individual levels of a multilevel decision problem. Using the framework, designers can perform efficient, robust co-design exploration. This is realized by employing the iSOM visualization tool to simultaneously explore the individual-level design spaces formulated using the rc-cDSP. iSOM visualization involves training iSOM using weight combinations corresponding to multilevel design scenarios of the rc-cDSP and goal values generated for these scenarios. Two-dimensional plots for the output goals across multiple levels are generated via iSOM. Using the simultaneous solution space visualization capability offered by iSOM, designers are further able to explore and seek common robust satisficing regions for the many goals across multiple levels, thereby facilitating co-design and the joint management of design conflicts and uncertainties. The framework supports designers in accounting for various soft and hard requirements across the design levels by facilitating their modeling in the rc-cDSP as goals and constraints, respectively. This allows consideration of any additional requirements relating to cost, production considerations, and process limitations during PMMP system design.

The framework's capability in supporting the above functionalities is demonstrated using an industry-inspired steel manufacturing process chain problem – HRR of steel. Using the framework, the co-design of the HRR PMMP system that involves the steel rod product, steel material, and the cooling process at two different levels - Design Levels 1 and 2, their interactions and inherent uncertainties are demonstrated. The design conflicts arising from the hierarchically related levels are managed by simultaneously exploring the solution spaces across Design Levels 1 and 2 to identify common robust satisficing solutions for the goals across the levels. In the HRR test problem, we consider model uncertainties in the YS design goal by assuming different mean, upper, and lower models. We assume that TS and HV functions are not subject to model uncertainties and thus consider their models mean models. The uncertainty associated with the function parameters of TS and HV are considered. This assumption is made to demonstrate the efficacy of the robust design constructs for various sources of uncertainties in the problem, namely model structure uncertainty (via EMI metric) and model parameter uncertainty (via DCI metric). The limitation of such an assumption is that the design solutions found will be sensitive to model variability since models are always abstractions of reality. The formulation of model uncertainty requires designers to have data sets that capture the variability of the function with respect to the design variables. This could be practically difficult for certain materials design problems with limited information. The integrated mean response model and prediction interval approach presented by McDowell and co-authors [34] allows the efficient estimation of the mean function model and prediction intervals, defining the upper and lower bounds if simulation-assisted or experimental data is available. Extending the current framework with efficient data-driven approaches to consider model uncertainty and its propagation across levels is a focus for future research.

The generic nature of the framework is made evident by the generic nature of the constructs and tools employed. Using the framework, we facilitate the robust co-design of multilevel PMMP systems characterized by many design goals requiring trade-offs at individual levels and hierarchical relations among the levels. From an ICME perspective, the CoDE-MU framework supports the need to consider the influence of manufacturing processing in materials design. This is achieved by facilitating the consideration of manufacturing processing decisions and their influences during PMMP systems design. The CoDE-MU framework can also facilitate location-specific materials design, a significant focus area in ICME. Location-specific materials design can be realized by supporting the designers to account for the influence of the manufacturing process to tailor material microstructure and properties at desired locations.

The proposed CoDE-MU framework can be further expanded to account for all the manufacturing processing decisions and their interactions by modifying the rc-cDSP formulation with additional levels. The changes to the rc-cDSP required to facilitate the same involve creating additional priority levels in the Preemptive formulation of the deviation function. Consequently, the multilevel design scenarios need to be modified to account for the new design levels in the PMMP system.

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CONFLICT OF INTEREST STATEMENT

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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APPENDIX A

In Table A1, we present the empirical models that relate the steel microstructure and composition with the steel rod properties. These models are employed in modeling the decision problem at Design Level 1, as described in Block B of Section 4. The YS_{lower}, YS_{mean}, and YS_{upper} models depict the uncertainties in the YS model, as described in Step A2, Block A of Section 4.

TABLE A1: Empirical models for mechanical property goals at Design Level 1

(T_{mf} = 700^{0}C, p= 6μm, t_{carb}= 0.025μm)

Mechanical Property	Empirical Model	Source
YS_{lower} $[\boldsymbol{f_2(x)}]$	$X_f(77.7 + 59.9[Mn] + 9.1(D_\alpha{*}0.001)^{-0.5}) + 478[N]^{0.5} + 1200[P] + (1 - X_f)(145.5 + 3.5S_0^{-0.5})$	Kuziac and co-authors (1997) [44]
YS_{mean} $[\boldsymbol{f_o(x)}]$	$63[Si] + 425[N]^{0.5} + X_f^{1/3}(35 + 58[Mn] + 17(0.001D_\alpha)^{-0.5}) + (1 - X_f^{1/3})(179 + 3.9S_0^{-0.5})$	Gladman and co-authors (1972) [42]

YS_{upper} [$f_1(x)$]	$62.6 + 26.1[Mn] + 60.2[Si] + 759[P] + 212.9[Cu] + 3286[N] + 19.7(0.001D_{\alpha})^{-0.5}$	Hodgson & Gibbs (1992) [43]
TS	$X_f(20 + 2440[N]^{0.5} + 18.5(0.001*D_{\alpha})^{-0.5} + 750(1 - X_f) + 3(1 - X_f^{0.5})\ S_0^{-0.5} + 92.5*[Si]$	Kuziac and co-authors (1997) [44]
HV	$X_f(361 - 0.357T_{mf} + 50[Si]) + 175(1 - X_f)$	Yada (1988) [45]

In Table A2, we present the empirical models that relate the steel microstructure and composition before cooling and the cooling processing parameters with the steel microstructure at the end of the cooling process. These models are employed in modeling the decision problem at Design Level 2, as described in Block B of Section 4.

TABLE A2: Empirical models for steel microstructure characteristics at the end of cooling at Design Level 2

Microstructure characteristics	Empirical Models	Source
D_{α}	$(1 - 0.45\varepsilon_r^{0.5}) *\{(-0.4 + 6.37*C_{eq}) + (24.2 - 59*C_{eq})\ CR^{-0.5} + 22*(1-\exp(-0.015*d_{\gamma}))\}$	Hodgson & Gibbs (1992) [43]
S_0	$0.1307 + 1.027[C] - 1.993[C]^2 - 0.1108[Mn] + 0.0305*CR^{-0.52}$	Kuziac and co-authors (1997) [44]
$X_{f\ eq}$	$1 - ([C] / (0.789 - 0.1671[Mn] + (0.1607[Mn]^2) - (0.0448[Mn]^3)))$	Kuziac and co-authors (1997) [44]
X_f	$X_{f\ eq} - 5.48(1-\exp(-0.0106CR)) - (0.723*(1-\exp(-0.0009d_{\gamma})))$	Kuziac and co-authors (1997) [44]
C_{eq}	$([C] + [Mn])/6$	Hodgson & Gibbs (1992) [43]