



Enabling sustainability-by-design with multi-disciplinary computer aided systems

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ARTICLE INFO

Article history:

Available online 20 May 2025

Keywords:

Eco-design methodology

Design optimization

Computer aided design (cad)

ABSTRACT

Sustainability-by-Design requires information and communication technologies (ICTs) capable of integrating design engineering, manufacturing processes, materials, and sustainability considerations. Currently, methodologies for assessing environmental sustainability, such as product life cycle assessment, are often implemented too late in the design process, reducing opportunities for early intervention. Integrating environmental sustainability modeling in computer-aided systems (CAx) allows engineers to concurrently evaluate trade-offs between technical performance and environmental impact, facilitating informed decision-making during embodiment design stages. Using a prosthetic device produced via material jetting additive manufacturing as case study, we demonstrate the transformative role of advanced CAx tools capable of analyzing trade-offs among competing objectives.

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1. Background to research

Product development is complex and multi-disciplinary. Effective management of complexity involves greater integration of various domains and developing advanced information and communication technologies (ICTs) to enhance computer-aided processes [1]. Today, engineering design and manufacturing generates vast amounts of data from initial design concepts to material testing, simulations, and manufacturing processes [2].

The careful storage, preparation, integration of data and derived models can revolutionize decision-making by uncovering complex interactions among coupled variables across disciplines [3]. Managing cross-disciplinary non-linear relationships effectively is challenging [4]. This is particularly evident in sequential engineering design approaches, where design choices are optimized within specific disciplinary boundaries without adequately considering their broader impacts, disciplinary couplings, and trade-offs [5].

The objective of this research is to demonstrate how computer aided systems' (CAx) intelligence can be enhanced by coupling interrelated functions between design engineering, manufacturing processes, material systems, and environmental sustainability [6]. The hypothesis is that a new wave of CAx systems must support our ability to explore and exploit cause-effects across disciplines [7]. This allows expanding engineers' design capabilities while embedding Sustainability-by-Design principles already at the embodiment design stages. Therefore,

it requires that datasets and models across computer design and simulation, material systems, manufacturing systems, environmental, and sustainability disciplines be fully connected with CAx [8].

The vision is to augment engineering capabilities for efficient decision-making by quantitatively uncovering disciplinary interrelationships and accounting for the ripple effects of engineering decisions on environmental sustainability from early stages, including product conceptualization to manufacturing.

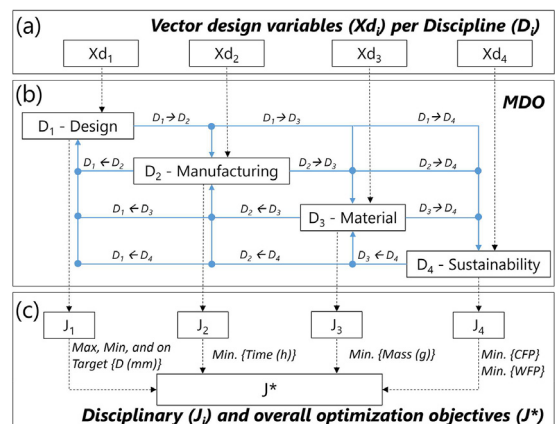


Fig. 1. Information and execution flow in the MDO problem formulation.

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2. Materials and methods

2.1. MDO framework and decomposition of disciplines

Model and data-driven surrogates and multidisciplinary design optimization (MDO) offer a solution to decompose and concurrently optimize multiple disciplines, allowing for a more holistic optimization at system-level. Fig. 1 shows how to graphically represent disciplinary interrelationships [9]. Fig. 1(a) shows the vector of design variables per discipline. Namely, X_{d1} for product design variables, X_{d2} for manufacturing, X_{d3} for material-related choices, and X_{d4} for sustainability related considerations. Fig. 1(b) shows how disciplines are decomposed into four domains (i.e., D_i). Specifically, D_1 for design, D_2 for manufacturing, D_3 for material, and D_4 for sustainability. Cross-disciplinary relationships are modelled by shared functions, constraints, and variables (i.e., $D_i \rightarrow D_j$). In turn, Fig. 1(c) shows how each discipline has its objective functions (i.e., J_i).

These objective functions act as inputs for the system-level performance evaluation and are used to compute the overall optimization objective function (i.e., J^*). To do so, high fidelity model-driven and data-driven surrogates are created via virtual and physical design of experiments (DOE), aiming to mathematically couple and solve the design to manufacturing workflow as an interrelated problem.

2.2. Sustainability-by-design: manufacturing process modeling

Sustainability-by-Design principles offer a strategic approach to embedding environmental, social, and economic sustainability into the design of products, systems, and services from the earliest stages, ensuring the organic inclusion of sustainability considerations. When considering the environmental impact, the approach translates into minimizing resource use, energy consumption, and waste from material extraction to product end-of-life [10]. Minimization of waste through enhanced material selection, engineering design choices, and manufacturing alternatives also ensures that emissions, toxic by-products, and waste are reduced throughout the product lifecycle [11].

However, *how can design engineers effectively predict the environmental sustainability impact of their decisions early in the design stage?* Current methodologies for calculating carbon footprint or conducting life cycle assessment (LCA) are typically applied too late in the process [1,12–14]. By the time these analyses are performed, decisions regarding geometry, materials, and manufacturing methods have already been finalized, reducing the opportunity for meaningful early intervention [15]. Such “post-mortem” approach highlights the need to integrate environmental sustainability assessment directly into CAx, to evaluate the trade-offs of engineering choices in real time. Fig. 2(a) describes the manufacturing process mapping, and the system boundaries considered in this research. The goal of the environmental impact assessment is to appraise environmental impact indicators, such as carbon and water footprint (CFP and WFP

respectively) of the product design considered, according to a “cradle-to-gate” approach, i.e., including the impact of extraction and refinement of raw materials until the shipment of the final product to the customer. The inventory of material and process data is sourced from the scientific literature, well-established databases (e.g., Ansys Granta Selector [16], Ecoinvent [17]) and first principles (i.e., conservation of mass and energy) coupled with experimental observations.

2.3. Case study: limb prosthetic socket design

Additive manufacturing (AM) enables fully digital workflows for personalized prosthetics that can be engineered using patient-specific anatomical data from computer tomography (CT) or magnetic resonance imaging (MRI) scans. Structural optimization and finite element analysis (FEA) techniques allow for balancing stiffness and lightweight design. Multi-material properties enable the creation of prosthetics with both rigid and soft zones within a single socket, enhancing comfort and performance [18]. In this case study, we developed a parametric computer aided engineering (CAE) model of a total surface bearing socket design, integrating FEA automation to optimize its mechanical properties based on socket geometry variables and material distribution, see Fig. 3. The FEA simulations evaluated the mechanical behavior of the prosthetic socket, focusing on the stresses at the stump-socket interface, where both pressure and shear stress must be managed to prevent skin breakdown and enhance patient comfort. Existing research indicates that pressures of up to 350 kPa and shear stress 85 kPa are common values to be employed [19].

2.4. Model and data-driven methods for MDO modeling

Product-design discipline (D1) employs a parametric FEA model-driven design automation. Fig. 2(b) shows the geometrical details of the socket, with varying width (w), depth (d), and height (h) dimensions. Additionally, the vector of product design variables (X_{d1}) comprises the soft region thickness (St) and rigid region thickness (Rt). Fig. 2(c) shows the complete prosthetic device, the socket soft region in contact with the skin and rigid region providing stiffness and structural support. While maintaining a constant thickness and material properties for the soft region, the design exploration focuses on varying Rt and V_f , affecting material properties, i.e., Young's modulus (E), yield strength (YS), density (ρ). Two key dependent variables are analyzed: the safety factor (S_f), calculated using the von Mises yield criterion to ensure structural integrity, and the maximum total deformation (D), which influences the socket's stiffness and flexibility. Optimization scenarios for ($J1$) require both minimization and maximization of D to obtain the most flexible socket design for increased comfort for early users or the stiffest socket possible for increase mechanical transmission of advance users. Inductive design, targeting, and programming D is also a possibility based on user preferences on prosthetic flexibility.

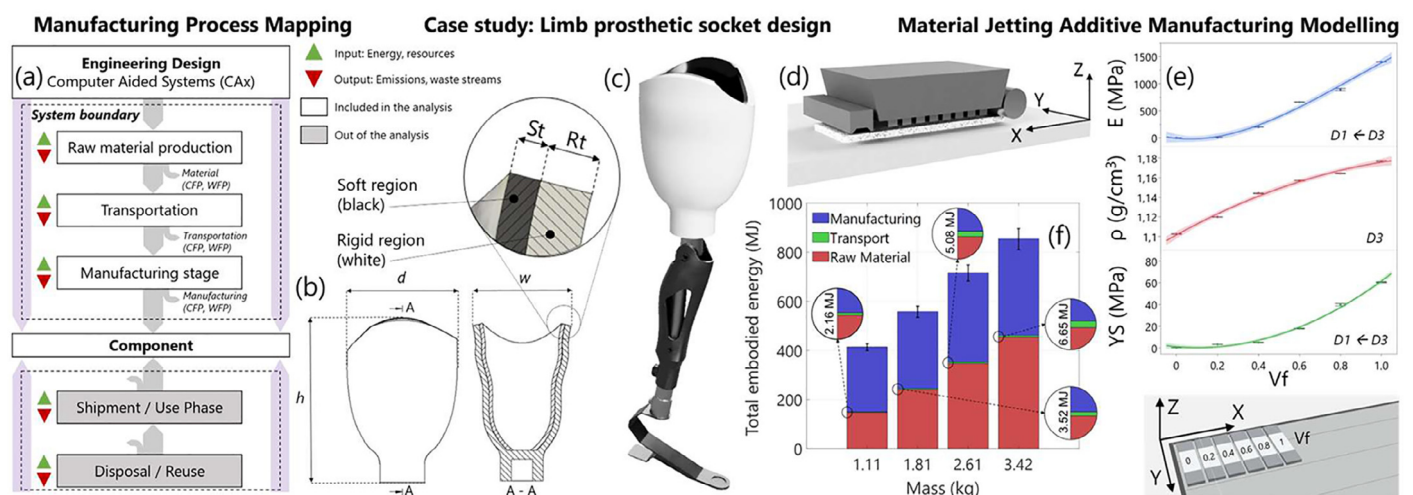


Fig. 2. Manufacturing process chain mapping, case study, and modelling.

Manufacturing discipline (D2) examines factors influencing manufacturing time (Mt) and energy consumption (EN). Mt was evaluated with a DOE comprising part height (H), build area (A), and average material volume fraction (Vf). To estimate Mt , 27 test trials were simulated using a CAM software. The disciplinary optimization objective ($J2$) aims at minimizing Mt that increase together with H and A . Electric current intensity during the material jetting process was measured using a clamp amperemeter at the wall socket. Current intensity was 7.75 ± 0.15 A in 44 experimental observations varying print volume [20]. The resulting model for total power consumption and energy of the manufacturing process was obtained by multiplying power by voltage and recorded experimental print time.

Material discipline (D3) uses a material jetting Stratasys J750 system, see Fig. 2(d). Tensile specimens with different volume fraction (Vf) were fabricated. 18 samples were tested to model E VS, while ρ required 12 observations for modeling. Material jetting combines two photopolymers—flexible TangoPlus (TP) and rigid VeroClear (VC)—to achieve a range of mechanical properties through varying Vf , where $Vf = 1 - Vf_{frango}$. (i.e., $Vf = 1$ is rigid VC with $E = 1230.3 \pm 7.9$ MPa and $Vf = 0$ is flexible TP with $E = 0.52 \pm 0.23$ MPa) [21]. Fig. 2(e) shows the best-fit regression models used as material homogenization for the FEA. The optimization objective ($J3$) is to minimize the mass of the socket design (M), noting that density—and thus M —increases with increased Vf .

Sustainability discipline (D4) investigates the CFP and WFP (i.e., blue and grey water consumption respectively) as environmental sustainability indicators, comprising main steps such as: raw material production, supply-chain transportation, and manufacturing process, see Fig. 2(a). The uncertainties consider different geographical locations of material and processes as well as variations in manufacturing practices.

Raw material production impacts were estimated considering Ansys Granta Selector [16] based on a specific carbon footprint 6.17–6.81 $\text{kg}_{\text{CO}_2\text{e}}/\text{kg}$ and water footprint 72.3–79.9 l/kg. Supply-chain transportation was assumed over a 500 km distance with a EURO 4, 7.5–16 ton truck emitting $2.5 \cdot 10^{-4}$ $\text{kg}_{\text{CO}_2\text{e}}/(\text{kg} \cdot \text{km})$ and consuming 0.236–0.402 l/(kg.km) of blue and grey water [22]. Although the assumptions related to the transportation step might in principle reduce the generality of the model, in practice it can be observed that the impact of transportation is by orders of magnitude less significant than raw material and manufacturing, see Fig. 2(f). Manufacturing environmental impacts were estimated converting the electric energy consumption to primary energy (i.e., assuming a primary energy factor 0.4) and considering an electric grid carbon footprint of 0.22 $\text{kg}_{\text{CO}_2\text{e}}/\text{kWh}$ [23] and water footprint of 1.308 l/TJ [24]. The material efficiency of the manufacturing process has been estimated ranging between 90%–98% [17,25, 26]. Ultimately, total embodied energy (EN) (i.e., raw material, transportation, and manufacturing) is modelled as a polynomial relationship between Mt and M . Minimizing the objective functions ($J4.1$) and ($J4.2$) leads to more environmentally sustainable designs.

For the modeling study, we used a surrogate modeling approach with third-order polynomial response surface approximations and two-factor interaction terms, refining the model through a stepwise regression to eliminate non-significant terms and balance complexity with predictive accuracy:

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^k \beta_{iii} x_i^3 + \sum_i \sum_j \beta_{ij} x_i x_j + \varepsilon$$

Where ε is the unobserved random error, β are the coefficients for each term (i.e., calculated by the least square method), x_i represent the independent variables. The interaction terms are represented by $x_i x_j$ and y is the dependent variable. The MDO process explores Vf and Rt to yield feasible and non-dominated solutions (J^*).

3. Results and discussion

3.1. Embodiment design and solution space exploration

Table 1 shows the disciplinary models, coupling models, and objective functions for this problem formulation involving material jetting AM. All the generated disciplinary data sets and surrogate models are openly available in GitLab [27].

Table 2 shows the formalized MDO problem formulation for the presented case study of a prosthetic socket design produced by material jetting additive manufacturing. To run the multi-disciplinary optimization, a Non-Dominated Sorting Genetic Algorithm (NSGA-II)

Table 1

Disciplinary models, coupling models, and objective functions.

MDO	Coupling functions and constraints	Fit
$D1 \leftarrow D3$	$E \text{ (MPa)} = -7.98 - 372.07 Vf + 2895.55 Vf^2 - 1134.03 Vf^3$	$R^2: 0.99$ RMSE: 60.71
$D1 \leftarrow D3$	$YS \text{ (MPa)} = 1.14 - 15.75 Vf + 76.33 Vf^2$	$R^2: 0.99$ RMSE: 2.07
$D2 \rightarrow D4$	$EN \text{ (MJ)} = 2.53 + 0.13 M + 328.13 Mt + 12.96 Mt^2$	$R^2: 0.99$ RMSE: 8.5E+5
$D1 \rightarrow D2$	$A \text{ (cm}^2\text{)} = 365.67 + 9.72 Rt - 0.27 Rt^2 + 0.005 Rt^3$	$R^2: 0.99$ RMSE: 0.91
$D1 \rightarrow D2$	$H \text{ (cm)} = 14.13 + 0.19 Rt$	$R^2: 0.99$ RMSE: 0.99
$D1 \rightarrow D3$	$Vol. r \text{ (cm}^3\text{)} = 166.2 + 73.64 Rt + 0.74 Rt^2 + 0.002 Rt^3$	$R^2: 1$ RMSE: 0.12
$D1$	$Sf = 1.65 - 0.25 Rt - 5.58 Vf + 0.01 Rt^2 + 2.54 Vf^2 + 0.401 Rt \cdot Vf$	$R^2: 0.99$ RMSE: 0.11
$D3$	$\rho \text{ (g/cm}^3\text{)} = 1.10 + 0.12 Vf - 0.04 Vf^2$	$R^2: 0.99$ RMSE: 0.1
$J1$	$D \text{ (mm)} = 218.29 - 14.26 Rt - 191.74 Vf + 0.27 Rt^2 + 68.59 Vf^2 + 3.71 Rt \cdot Vf$	$R^2: 0.89$ RMSE: 8.36
$J2$	$Mt \text{ (h)} = -15.91 + 2.71 H + 0.03 A + 4.13 Vf - 0.01 A^2 + 0.01 H \cdot A - 0.637 H \cdot Vf$	$R^2: 0.98$ RMSE: 5.57
$J3$	$M \text{ (g)} = (Vol. r) \times (\rho_{Vf(i)}) + (Vol. s) \times (\rho_{Vf(o)})$	$R^2: 0.99$ RMSE: 0.1
$J4.1$	$CFP \text{ (kg}_{\text{CO}_2\text{e}}\text{)} = 0.44 + 1.51E-7 EN + 0.01 M$	$R^2: 0.99$ RMSE: 0.05
$J4.2$	$WFP \text{ (m}^3\text{)} = 0.03 + 1.04E-8 EN + 0.01 M$	$R^2: 0.99$ RMSE: 0.01

is used as a solution space exploration engine [28]. Fig. 3(a) shows the process diagram including inputs (i.e., design variables Rt and Vf), MDO process with the automations between CAX, outputs (i.e., D , Sf , Mt , M , CFP, and WFP), and optimization objectives and constraints.

The results show that engineering decisions at the material micro-scale (i.e., Vf) and product design choices (i.e., Rt) had a ripple effect on concurrent disciplines including CFP and WFP environmental sustainability implications. Fig. 3(b) shows one of the explored combinations of variables for the socket product design and the resulting total deformation. Fig. 3(c) shows the feasible design space with Rt and Vf as a function of the margin of safety (Sf) used as inequality constraint function. Certain combinations of Vf and Rt would provide negative values for Sf . Thus, non-feasible solutions as the socket design would yield.

3.2. Detailed design and solution space exploitation

The detailed design requires concurrent optimization of all objective functions (i.e., Ji). The Pareto front (PF) refers to a set of solutions that are non-dominated with respect to each other in a multi-objective optimization problem. In mathematical terms, point $x^* \in F$ (where F refers to all the feasible solutions) is a Pareto optimal point if there is no other feasible point x that can reduce any criterion without simultaneously increasing at least one other criterion. This means that x^* achieves a balance in which any improvement in one objective would require a trade-off in another. Fig 3(d) shows the 3D scatter plot of feasible and non-dominated solutions. The results

Table 2

MDO problem formulation.

Find	
Engineering design subsystem level variables: Vf and Rt	
Satisfy	
Inequality constraint:	Goals (objective functions):
$Sf \geq 0$	(J1) Max or Min $\{D \text{ (mm)}\}$: Def.
Equality constraint:	(J2) Min $\{Mt \text{ (h)}\}$: Manufacturing time
$St \text{ (mm)} = 6$	(J3) Min $\{M \text{ (g)}\}$: Part weight
$\rho_{Vf(o)} = 1.12 \pm 0.06 \text{ g/cm}^3$	(J4.1) Min $\{CFP \text{ (kg}_{\text{CO}_2\text{e}}\text{)}\}$: Carbon FP
$Vol. s = 490.9 \text{ cm}^3$	(J4.2) Min $\{WFP \text{ (m}^3\text{)}\}$: Water FP
Bounds	
Product-design $D1 \text{ (Xd1)}$:	Material subsystem $D3 \text{ (Xd3)}$:
$5 \leq Rt \text{ (mm)} \leq 25$	$0 \leq Vf \leq 1$
Manufacturing subsystem $D2 \text{ (Xd2)}$:	
$0 \leq A \text{ (cm}^2\text{)} \leq 1911$	
$0 \leq H \text{ (cm)} \leq 20$	
System-level optimisation objective (J^*):	
An optimal set of feasible and non-dominated solutions for:	
Scenario #1 $\rightarrow$ Min. $\{CFP, WFP\}$; Min. $\{D \text{ (mm)}\}$; while $\{Sf \geq 0.5\}$	
Scenario #2 $\rightarrow$ Min. $\{CFP, WFP\}$; Max. $\{D \text{ (mm)}\}$; while $\{Sf \geq 0.5\}$	

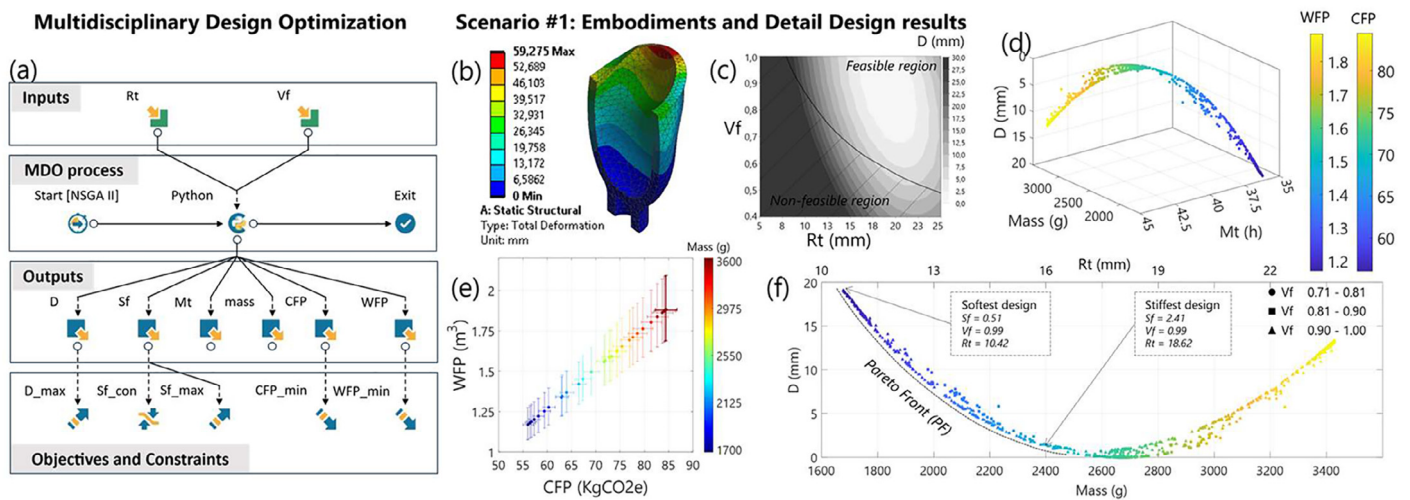


Fig. 3. MDO and results at embodiment and detail design stages.

demonstrate that the stiffer the prosthetic required the higher the M , Mt , as well its environmental footprint. Fig 3(e) shows the linear relationship between WFP and CFP with the mass of the product. It can be observed that WFP results are affected by a higher degree of uncertainty. Ultimately, Fig. 3(f) shows the PF for optimal results. In scenario #1 (i.e., min. CFP, WFP, and D to obtain the stiffest design, while $Sf \geq 0.5$) leading to a range of solutions. For example, the stiffest solution of the socket (i.e., $D = 1.01$ mm) will come at the cost of $Mt = 37.45$ h and $M = 2.40$ kg. The resulting environmental cost will be $WFP = 1.27$ m³ and $CFP = 60.15$ kgCO_{2e}. On the other hand, the softest solution (i.e., $D = 19.01$ mm) will lead to $Mt = 36.24$ h and $M = 1.69$ Kg with a $WFP = 1.17$ m³ and $CFP = 56.04$ kgCO_{2e}. The level of stiffness can be predefined allowing an inductive design approach. Target values for D accommodate patient needs, leading to different optimal material, manufacturing, and sustainability disciplinary implications.

4. Conclusions

Despite substantial challenges, engineers often attempt—sometimes successfully—to achieve optimal designs by manually enhancing concurrent design processes. A new generation of CAX should integrate new functionalities to predict environmental sustainability impact already at early embodiment design stages.

Generative and parametrized CAD-CAE design and simulation tools can automate the assessment of geometrical and material changes in mechanical performance. Simultaneously, CAD-CAM interfaces can be to estimate manufacturing time. Resulting product descriptors, such as mass and manufacturing time per each generated design can be coupled with total embodied energy and sustainability models to assess the resulting environmental impact. Interoperability among CAX systems requires cross-domain data exchange formats, integration with digital-twin frameworks [29], and alignment with Digital Product Passports initiatives and related regulatory efforts [30,31]. With this case study, we demonstrate how interrelated functions between environmental sustainability and engineering design couple with material systems and manufacturing process chains. The methodology and subsequent results show how it is possible to explore and exploit trade-offs between disciplines while embedding Sustainability-by-Design principles already at early design stages. Custom developed middleware interfaces enabled communication between engineering disciplinary CAX systems. Existing approaches to account environmental impact rely on "ad-hoc", repetitive or simplistic studies using general-purpose Life Cycle Assessment (LCA) tools. These prove inefficient in industrial contexts, as they may fail to capture the full complexity of multidisciplinary design of material and manufacturing relationships for early intervention.

While the entire product design discipline is inherently "problem-centered", the presented methodology, though applied to the prosthetic case, has general validity. Once the material systems and the manufacturing process chains—incorporating energy consumption,

environmental footprint, and other sustainability indicators—are modeled, they can support other design problems. For example, if a new design problem emerges, the material, manufacturing, and sustainability surrogates can be used in the CAX to assist in decision-making. This research is limited to modeling a single material system and material jetting AM, formulated as a low-dimensional problem centered on the prosthetic case study, using a polynomial response surface approximation. Future research is planned to develop, test, and model additional case-studies, material systems, and diverse multi-stage manufacturing process chains. In return, we foresee the need for deep learning and artificial intelligence methods to capture the complexity in higher dimensionality spaces including additional environmental sustainability metrics in cradle-to-gate and cradle-to-cradle analysis methods. The current technological and economic landscape presents an opportunity to develop a new class of multidisciplinary computational design environments. While this is an ambitious endeavor, embedding environmental sustainability at embodiment design stages has the potential to achieve significant gains. With improved CAX tools, engineers can produce multi-disciplinary optimal designs. In essence, providing advanced tools tailored to modern needs would naturally foster a design process that yields improved, more sustainable, and robust solutions, while enabling earlier, integrated, and more comprehensive trade-off explorations considering economic, social, and environmental sustainability.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Iñigo Flores Ituarte: Writing – review & editing, Writing – original draft, Visualization, Resources, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Emanuele Pagone:** Writing – review & editing, Validation, Methodology, Formal analysis. **Amirmohammad Daareyni:** Writing – review & editing, Software, Methodology, Formal analysis, Conceptualization. **Samniroshan Thayapararajah:** Software, Methodology, Formal analysis. **Guido Tosello:** Writing – review & editing, Validation, Supervision, Project administration, Conceptualization.

Acknowledgments

This work was supported by the project D2M (346874) Research council of Finland - Academy Research Fellow program.

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Thayapararajah, Samniroshan; Tosello, Guido**

2025

Elsevier

<https://doi.org/10.1016/j.cirp.2025.03.019>

Ituarte IF, Pagone E, Daareyni A, et al., (2025) Enabling sustainability-by-design with multi-disciplinary computer aided systems. CIRP Annals, Volume 74, Issue 1, 2025, pp. 209-213