

Luo, Julia, Candia Jorquera, Juan Ramon and Ball, Peter David (2026) A system-of-systems framework for Digital Twin enabled Real-Time Sustainability Reporting. International Journal of Production Research.

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To cite this article: Yujia Luo , Juan Ramón Candia & Peter Ball (29 Jul 2026): A system-of-systems framework for digital twin-enabled real-time sustainability reporting, International Journal of Production Research, DOI: [10.1080/00207543.2026.2703757](https://doi.org/10.1080/00207543.2026.2703757)

To link to this article: <https://doi.org/10.1080/00207543.2026.2703757>



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A system-of-systems framework for digital twin-enabled real-time sustainability reporting

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ABSTRACT

The convergence of Industry 5.0 imperatives, sustainability challenges, and compulsory reporting standards necessitate advances in manufacturing analysis. Digital Twins (DTs) enable real-time manufacturing monitoring and optimisation, yet remain disconnected from corporate sustainability reporting (SR). This separation restricts leveraging operational data for mandatory disclosures and seeking operational improvements from sustainability reporting insights. DT research has predominantly focused on energy efficiency, with limited attention to broader environmental dimensions. We address this gap by developing a System-of-Systems framework integrating operational DTs with SR requirements. The gap, identified through literature analysis, is confirmed using expert interviews. We identify data mismatches between DT systems with process-level data and SR using periodic, facility-level data. Applying System-of-Systems theory, we develop a four-step framework (Mapping, Matching, Measuring, Modelling) enabling systematic translation between two independent systems. The framework demonstrates how manufacturing systems DTs can both supply and respond to SR outputs. Examples drawn from interviews, a simplified manufacturing system, and an illustrative SR standard demonstrate applicability. The outcome is a structured approach for integrating DTs to support SR generation, and for SR insights to inform DT-enabled operational scenarios for performance enhancement. The contribution of the DT–SR framework lies in both modelling advancement and management practice.

ARTICLE HISTORY

Received 27 March 2025
Accepted 25 June 2026

KEYWORDS

Digital twins; sustainability reporting; manufacturing systems; system-of-systems theory; Industry 5.0

1. Introduction

The environmental footprint of manufacturing is growing, with resource consumption exceeding 50% of Earth's regeneration capacity (Li et al. 2020) of which industry globally accounts for 55% (Mawson and Hughes 2019). Rising population and consumption will further strain ecosystems (Garetti and Taisch 2012; Li et al. 2020).

Market demands, regulations, and corporate sustainability goals drive the need for better monitoring to balance productivity with environmental responsibility. Strategies to cut impacts include minimising waste, and optimising energy use (Larreina et al. 2013). Sustainability is recognised as a major challenge in industrial engineering (Karwowski et al. 2025) and key to manufacturing development goals (Blandino and Montagna 2025; Li et al. 2020).

Pursuing sustainability requires a systems perspective across the supply chain. Balancing environmental and social factors demands a life-cycle perspective (Li et al. 2020). Industry 4.0 technology focus (Shojaeinasab

et al. 2022) has evolved to Industry 5.0 prioritisation of sustainability, human-centricity, and resilience (Ivanov 2024; Xu et al. 2021; Yuan et al. 2024). With human well-being and ecological emphasis (Longo, Padovano, and Umbrello 2020), it supports a 'Techno-Social Revolution' that integrates efficiency with value-driven decision-making (Longo, Padovano, and Umbrello 2020; Xu et al. 2021).

Historically confined to engineering optimisation, the digital twin (DT) scope has broadened to represent the entire system lifecycle from conceptual design and manufacture to operation, maintenance, and decommissioning (Wang et al. 2023). DTs support environmentally sustainable business practices and circular economy (CE) principles across the lifecycle (Fosso-Wamba et al. 2026; Li et al. 2020) through optimising material usage, and energy consumption and minimising waste (Tagliabue et al. 2021).

Research, however, misses opportunities given the machine energy focus rather than broader carbon emissions and social impacts (Jiang et al. 2021; Tagli-

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 Supplemental data for this article can be accessed online at <http://dx.doi.org/10.1080/00207543.2026.2703757>.

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abue et al. 2021). The literature is limited to technology-orientation which neglects business-oriented viewpoints to link technology to auditable compliance (Kumbhar, Ng, and Bandaru 2023; Lin, Liu, et al. 2024). DTs aid operational efficiency but lack the strategic sustainability focus (Ivanov 2023a, 2024) and integration with corporate sustainability performance (Blandino and Montagna 2025; Ma, Qi, and Tao 2024). Prior work has not established protocols for translating dynamic operational data into the sustainability metrics required by international standards, including the Global Reporting Initiative (GRI) Standards (e.g. GRI 302: Energy), the Greenhouse Gas Protocol Corporate Standard, the International Sustainability Standards Board (ISSB) standards (International Financial Reporting Standard S2), and the European Sustainability Reporting Standards under the Corporate Sustainability Reporting Directive (CSRD).

Satisfying sustainability reporting requirements using DTs faces technical and organisational barriers. The regulatory landscape, specifically the introduction, for example, of the CSRD mandates stringent disclosures for global enterprises, within and beyond the European Union (European Parliament 2024). This mandate transforms SR from a voluntary exercise into a legal, financial obligation. Manufacturing systems are adapting with digital tools like DTs to support sustainability. This study investigates how DTs could enhance sustainability reporting (SR), positioning the two so they are both input to and an output of performance improvement. The research question is: 'How could manufacturing digital twins (DTs) facilitate and enhance corporate sustainability reporting (SR)?'

The present paper extends a preliminary version of the framework (Luo, Candia, and Ball 2026) through full operationalisation of the four-step framework and empirical grounding from ten expert interviews across seven organisations. The paper is structured as follows: Section 2 details the literature review on systems theory, DTs, SR and data integration to identify research gaps. Section 3 presents the methodology including the results from interviews to verify and enhance the literature findings. Section 4 details the development of a system-of-systems (SoS) framework linking DTs with SR which is then applied in Section 5 in a four-step approach: mapping, matching, measuring, and modelling. Section 6 and 7 respectively discuss the findings and conclude with contributions, managerial implications and future research.

2. State-of-the-art review

This literature review first considers the lens of system theories for subsequent analysis. The two systems of (1)

manufacturing and associated DTs and (2) SR are examined in detail to establish knowledge gaps. Then data requirements for manufacturing DTs and SR systems are reviewed to uncover how they are, or not, applied. Subsequently, the SoS principle of emergent capabilities illustrates the necessity and benefits of DT-SR integration. Finally, the gaps are assembled to confirm the research question posed.

2.1. Theoretical foundation: SoS theory for DT in Industry 5.0

System-of-Systems (SoS) theory contends that complex systems can be decomposed into autonomous yet interdependent subsystems that exhibit emergent behaviour through their interactions (Maier 1998). For manufacturing, SoS principles include: (1) functional autonomy of subsystems; (2) managerial independence of subsystems; (3) evolution of systems over time and (4) emergent behaviour where system-level capabilities arise from subsystem interactions (Maier 1998). DTs as a feature of Industry 5.0, defined by Ivanov (2023b) as a viability-based integration of resilience, sustainability, and human-centricity, can be framed using SoS to capture the manufacturing system as interconnected, self-organising subsystems, ensuring flexibility, responsiveness, and emergent intelligence (Blandino and Montagna 2025; Ghobakhloo et al. 2026; Karwowski et al. 2025).

DT technology has evolved from a virtual representation synchronised with physical systems (Grieves and Vickers 2016) to a broader scope of Industry 4.0 and 5.0 (Xu et al. 2021). DT definition is ambiguous (Bitencourt, Wooley, and Harris 2025) with some implementations lacking bidirectional data synchronisation between physical and virtual systems (Bitencourt, Wooley, and Harris 2025). Maturity models are needed to acknowledge DTs exist along a capability spectrum rather than as binary implementations (Kober et al. 2025). The International Organization for Standardization (ISO) defines a DT as 'a fit-for-purpose digital representation of an observable manufacturing element with synchronization between the element and its digital representation' (ISO 2021).

A DT can be conceptualised as a set of virtual information constructs that mimics the structure, context, and behaviour of a system while being dynamically updated with data from its physical twin to inform decisions (Grieves and Vickers 2016). In the context of Industry 5.0, human-centricity, sustainability, and resilience are paramount (Ivanov 2023b). These high-fidelity representations enhance operational efficiency, facilitate predictive maintenance, and support strategic decision-making (Flores-García et al. 2025) and resilience (Fosso-Wamba

et al. 2026). Critically, DTs may need to extend operational efficiency objectives to encompass broader sustainability and social responsibility (Karwowski et al. 2025; Longo, Padovano, and Umbrello 2020).

A manufacturing system can be conceptualised as a composite of interdependent, nested systems (Ball et al. 2009). This hierarchical structure manifests across multiple levels from individual machines and workstations (micro-level), through production lines and cells (meso-level), to complete factories and supply chains (macro-level) (Psarommatis, May, and Azamfirei 2024). DTs operating at each level are not only autonomous but can be further decomposed into sub-subsystems to capture granularity. This nested configuration permits micro-level monitoring while capturing emergent, system-level performance – a characteristic essential for translating operational sustainability impacts into enterprise-level reporting metrics.

Manufacturing DTs thus exemplify SoS principles: individual elements (machine twins, process twins, product twins) operate autonomously yet remain interconnected (De Carolis et al. 2025), collectively capturing system behaviour across the lifecycle from design through manufacture to decommissioning.

The SoS framing is well suited to sustainability. Sustainability performance inherently emerges from the interaction of multiple operational subsystems, including machine energy consumptions, material flows, waste generation across production stages, and human well-being in work environments. Reductionist approaches that optimise individual subsystems may produce local improvements without system-level sustainability gains or even generate unintended negative consequences elsewhere (Psarommatis, May, and Azamfirei 2024). As theoretical grounding, SoS acknowledges this complexity for investigating how to orchestrate DTs for emergent sustainability performance at the enterprise level.

2.2. System 1: manufacturing digital twins

A manufacturing DT provides insights (Mantravadi and Møller 2019; Xu et al. 2021) and autonomously optimises in real-time (Shojaeinasab et al. 2022). Applications span (1) general; (2) metal parts; (3) electrical equipment; (4) transportation equipment; (5) aerospace; (6) additive; and (7) energy (oil and gas, pharmaceuticals, and battery) (Bitencourt, Wooley, and Harris 2025). Applications include specific functions such as design and prototyping (Huang, Wang, and Yan 2022; Liu et al. 2022), production planning (Badakhshan and Ball 2023, 2024; Lin, Liu, et al. 2024; Luo and Ball 2025), quality control (Li et al. 2023; Liu et al. 2021), predictive maintenance (Wang,

Zhang, and Zhong 2020) and human-robot interactions (Yuan et al. 2024). Further contributions demonstrate the expanding scope of manufacturing DT applications towards intelligent and resilient DT system design (Finco et al. 2026), including knowledge-driven DT manufacturing cells (Zhou et al. 2020); cognitive DT frameworks addressing vision, challenges, and opportunities (Zheng, Lu, and Kiritsis 2022); shop-floor reconfiguration for uncertainty management (Zhang et al. 2025); and manufacturing service collaboration (Cheng et al. 2025).

Sensor technologies enable real-time process measurement for production optimisation (Kaewunruen, Peng, and Phil-Ebosie 2020; Luo and Ball 2025). The data architecture of DTs typically comprises five layers: (1) Physical: sensors, actuators, and equipment generating operational data; (2) Edge: local data preprocessing and filtering to reduce transmission loads; (3) Platform: cloud or enterprise systems for data storage, integration, and management; (4) Analytics: algorithms for simulation, optimisation, and prediction; (5) Application: user interfaces and decision support tools (Liu, Zheng, and Bao 2024). Integration of heterogeneous data sources remains problematic – machine data typically uses proprietary protocols, enterprise systems use different standards (e.g. ISA-95), and sustainability data in turn resides separately with incompatible formats (Tufano 2023).

Gaps remain. DTs can contribute to sustainability goals like material optimisation, energy efficiency, and waste reduction (Larreina et al. 2013; Tagliabue et al. 2021), yet sustainability benefits are often incidental rather than intentional (Tao et al. 2022). DT focus on energy management overlooks broader sustainability metrics like carbon emissions and social impact (Jiang et al. 2021; Ma, Qi, and Tao 2024; Tagliabue et al. 2021). This limited scope reflects a disconnect of purpose-built DTs for operational objectives (efficiency, quality, throughput) rather than for sustainability reporting or strategic sustainability management. Moreover, DT implementations are confined within operations, lacking connections to the enterprise-level sustainability management systems responsible for corporate reporting (Bitencourt, Wooley, and Harris 2025). Empirical work reinforces this boundary. Kamble et al. (2022) propose a DT sustainability framework for supply chains addressing carbon and resource flows but do not translate operational data into formal disclosure metrics (GRI, ESRS, ISSB). This research addresses the gap of a systematic approach to translate granular, real-time manufacturing DT data into enterprise-level sustainability reporting metrics for strategic decision-making and stakeholder reporting.

2.3. System 2: sustainability reporting

Sustainability Reporting (SR) operates as a distinct subsystem within an enterprise. SR draws from the manufacturing DT system (i.e. System 1) through data aggregation and synthesis and to provide strategic insights for improvement (Juvvala, Sangle, and Tiwari 2025; Messina, Eslami, and Castilla 2025) across environmental, social, and economic performance (Abeysekera 2022). Examples include ISO 14001, ISO 50001, Leadership in Energy and Environmental Design (LEED), Eco-Management and Audit Scheme (EMAS), UN Global Compact, Global Reporting Initiative (GRI), Carbon Disclosure Project (CDP), Task Force on Climate-related Financial Disclosures (TCFD), Task Force on Nature-related Financial Disclosures (TNFD). More recently, the ISSB has published IFRS S1 and S2, consolidating investor-focused disclosure requirements across earlier voluntary schemes (ISSB 2023). The GHG Protocol Corporate Standard, while not a disclosure framework per se, underpins emissions accounting across virtually all of the above and warrants explicit recognition as a foundational methodological reference. Wang et al. (2026) confirm that ESG integration in supply chains is increasingly expected of manufacturing enterprises, reinforcing the relevance of the DT-SR integration this paper addresses.

SR standards driven by investor demands, regulatory pressures, and stakeholder expectations (Osobajo et al. 2022) share common elements, including reporting on energy, emissions, water, waste, materials, worker conditions, community impacts, and governance, but differ significantly in scope, boundary definitions, metrics, and calculation methodologies. This complexity creates challenges for manufacturers that different reporting requirements demand different data, calculated differently, from different system boundaries. A single operational data point (e.g. kilowatt-hours of electricity consumed) may feed into multiple reporting metrics (Scope 2 emissions, energy intensity ratios, renewable energy percentage), each requiring different denominators, conversion factors, and contextual data.

Despite the evolution of reporting frameworks, significant limitations constrain SR effectiveness for driving operational sustainability. First, most SR operates on annual or quarterly reporting cycles, aggregating historical data at fixed intervals (Silva, Nuzum, and Schaltegger 2019). Second, SR frameworks typically require facility-level or company-level aggregate metrics, losing the process-level and machine-level granularity where operational improvements are actually implemented (Osobajo et al. 2022). Third, sustainability data often relies on manual rather than system collection, estimation and allocation methods which lead to data quality

concerns (Silva, Nuzum, and Schaltegger 2019). Fourth, SR systems typically operate separately from manufacturing execution systems, enterprise resource planning systems, and operational technologies (Tagliabue et al. 2021).

These limitations reveal a fundamental architectural problem that SR systems were designed for external stakeholder communication and compliance, not for internal operational optimisation. SR receives operational data but does not drive improvements in environmental, social, and governance (Nguyen et al. 2022; Perotti et al. 2024). DTs, conversely, are configured for internal operational optimisation, not external sustainability reporting. This research considers how these two systems (designed for different purposes, operating at different timescales and granularities, using different data structures) can be systematically integrated to support system level optimisation where DTs enable real-time SR and SR insights drive DT-enabled operational adaptation.

2.4. Data for manufacturing digital twins

DTs are typically applications and scenario specific (Bhandal et al. 2022; Nguyen et al. 2022). This purposeful scoping explains why no DT implementations have been reported that support corporate sustainability reporting as a primary design objective. The complexity of integrating diverse sustainability metrics spanning environmental, social, and governance dimensions while maintaining operational fidelity could substantially increase development and validation time.

Manufacturing systems, and their DTs, exhibit complexity arising from dynamic interactions between humans, technology, materials, and processes within constrained physical and temporal boundaries (Aheleroff et al. 2021). To unravel DT applications (Newrzella, Franklin, and Haider 2021), researchers have proposed various taxonomies for categorising DT data dimensions (Liu et al. 2022, 2024; Ma, Qi, and Tao 2024). To relate DT data with SR, data categorisation is critical to find linkages between manufacturing operations and company sustainability metrics. It must reflect system scale (depth) and scope (breadth) to evaluate manufacturing system sustainability performance (Wang, Zhang, and Zhong 2020). It should include product, material, machine, process, human/operator, and system dimensions (Huang, Wang, and Yan 2022; Lin, Chen, et al. 2024; Liu et al. 2022, 2024; Ma, Qi, and Tao 2024; Wang et al. 2019; Yuan et al. 2024). Table 1 provides the commonly used perspectives with examples provided to prepare for later DT and sustainability performance indicators alignment.

Most implementations sidestep these integration challenges by limiting scope to controlled subsets, including

Table 1. Common data categories of manufacturing DTs.

Dimension	Categories	Subcategories
Scope and Scale	Product	Product design files, material composition data, product lifecycle information
	Material	Supplier data, material properties, material certifications
	Machine	Machine specifications, maintenance records, energy consumption data
	Process	Process flow diagrams, production schedules, quality control data
	Human/Operator	Employee training records, skill sets, performance data, safety records
	System	Plant layout, supply chain information, environmental impact assessments

Source: update from Newrzella, Franklin, and Haider (2021), Tao et al. (2022), and Wang et al. (2023).

using simulation with assumed data availability rather than real-time feeds, focusing on single machines or processes rather than system-wide integration, or conducting proof-of-concept demonstrations in laboratory environments with simplified data (Bitencourt, Wooley, and Harris 2025). This explains the scarcity of DT implementations addressing enterprise-level SR. While manufacturing DTs can theoretically provide comprehensive real-time data for sustainability assessment, current implementations lack the data architecture, semantic mapping, and integration mechanisms necessary to translate DT data into standardised sustainability reporting metrics.

2.5. Data for sustainability reporting

Sustainability reporting (SR) standards define data requirements organised hierarchically for external accountability. For instance, CSRD requires sustainability statements with increasing assurance equivalent to financial audit standards (European Parliament 2024).

The European Sustainability Reporting Standards (ESRS), representing the most comprehensive and stringent mandatory framework currently in force, exemplifies this structure (European Parliament 2024). Table 2 outlines the key aspects included. ESRS comprises cross-cutting standards (governance and disclosure requirements applicable across all topics), topical standards addressing environmental (E1–E5: climate, pollution, water, biodiversity, circular economy), social (S1–S4: workforce, value chain, communities, consumers), and governance dimensions (G1: business conduct), with sector-specific standards under development tailored to industry characteristics (EFRAG 2024). Each topical standard defines metrics at multiple levels of specificity: broad topics (e.g. climate change), sub-topics (e.g. energy consumption, GHG emissions), and specific metrics (e.g. total energy consumption in MWh disaggregated by renewable/non-renewable sources). Appendix 1 provides comprehensive mapping of ESRS topics and sub-topics.

Table 2. European sustainability reporting standards (ESRS).

Category	Standard	Content / Sustainability Themes
Cross-cutting standards	ESRS 1 ESRS 2	General requirements General disclosures
Topical standards	ESRS E1	Climate change
	ESRS E2	Pollution
	ESRS E3	Water and marine resources
	ESRS E4	Biodiversity and ecosystems
	ESRS E5	Resource use and circular economy
	ESRS S1	Own workforce
	ESRS S2	Workers in the value chain
	ESRS S3	Affected communities
	ESRS S4	Consumers and end-users
	ESRS G1	Business conduct

Note: E: Environment, S: Social, G: Governance.

Source: European Parliament (2024).

Appendix 2 details specific metrics for ESRS E1 Climate Change as an illustrative example.

Despite growing data collection sophistication, current data architectures have limited links to operational performance management. SR data collection for annual aggregate disclosure is insufficient for operational optimisation. Data can be aggregated by manual calculation and spreadsheet consolidation from diverse sources with conversion methodologies (e.g. emission factors and allocation assumptions). For instance, emissions are calculated annually using standardised emission factors rather than measured directly from operations. Water and energy consumption derives from aggregated utility bills at facility-level (monthly or quarterly intervals) with minimal operational granularity. This aggregated, periodic, calculated approach provides verification and auditability for external stakeholders but limits granular operational connections (Osobajo et al. 2022).

While not SR design flaws, any consequential operational improvement is constrained. Manufacturing DTs capture operational data at granularities and frequencies different from, yet complementary to, SR requirements. DT data contains the operational genesis of sustainability impacts (Li et al. 2020). For instance, rather than annual facility totals, DTs generate continuous streams of machine-level, process-level, and operational-level data such as energy consumption in kilowatt-hour increments at machines and material flows at production lines (Nguyen et al. 2022).

2.6. SoS theoretical mechanisms: enabling emergent DT-SR capabilities

Maier's (1998) SoS principle captures emergent behaviours arising from interactions between constituent systems that neither system produces independently. SoS provides the theoretical framework for understanding how DT and SR systems can be integrated to generate emergent capabilities. DTs and SR systems exemplify

SoSs where autonomous systems with distinct purposes with independent governance, management, organisational placement, and design objectives. Neither system depends on the other for functionality. This operational autonomy means DT-SR integration need not demand organisational consolidation, system redesign, or subordinating one system objectives to another. Rather, it requires designing interfaces, namely data exchange mechanisms, calculation procedures, feedback pathways, through which autonomous DT and SR systems coordinate toward bidirectional optimisation.

SoS theory suggests differences between DT operational requirements and SR reporting requirements are not barriers to integration but rather delineate the interface design space, where four emergent capabilities could be potentially generated:

Real-time sustainability visibility. Potential for continuous calculation of sustainability, transforming sustainability from a lagging indicator (historical performance) to a real-time control signal.

Sustainability diagnostic capability. Integration could enable hierarchical drilling down from facility-level deviations to operational causes. For instance, when facility energy consumption exceeds targets, operations staff could identify which equipment or processes was the driver.

Predictive sustainability management. Rather than reacting to sustainability deviations, organisations could explore how anticipated production changes affect sustainability performance, test operational adjustments before implementation, and proactively manage sustainability impacts.

Bidirectional optimization capability. Emerging from DT-SR integration, DT optimization algorithms incorporate SR targets as constraints (ensuring efficiency gains do not increase environmental impact or social disruption). SR insights identify high-leverage opportunities where operational changes generate disproportionate sustainability benefits.

These emergent capabilities arise from DT-SR connection but exist in neither system alone. Figure 1 captures the theoretical mechanisms of SoS emergent capabilities from DT-SR integration.

2.7. Research gap in data and reporting

Despite substantial research on manufacturing productivity and sustainability reporting, investigation of architectures integrating these domains is limited. While DTs are increasingly applied to enhance energy efficiency, predictive maintenance, and overall operational performance (Flores-García et al. 2025; Grieves and Vickers 2016), their potential to transform SR has not been realised, with a notable gap in extending their utility to broader sustainability indicators (Juvvala, Sangle, and Tiwari 2025; Messina, Eslami, and Castilla 2025).

Sections 2.4 and 2.5 confirmed that while manufacturing DT evaluation and sustainability reporting metrics address related phenomena (energy use, material flows, waste generation) (De Carolis et al. 2025), no systematic methodologies exist for translating granular DT operational data into standardised SR metrics (Guandalini 2022; Juvvala, Sangle, and Tiwari 2025; Messina, Eslami, and Castilla 2025).

SoS theory, while well-established for complex distributed systems (Maier 1998; Psarommatis, May, and Azamfirei 2024), has not been theoretically developed for DT-SR integration; practitioners consequently lack actionable implementation frameworks (Fosso-Wamba et al. 2026). The literature reveals DT frameworks for operational applications (Ivanov 2024; Liu et al. 2021) and SR frameworks for disclosure (GRI, ESRS, ISSB), but no frameworks connecting these domains. This gap is notable given that ISO 23247:2021 provides a reference architecture for manufacturing DTs and the GHG Protocol defines the dominant emissions accounting methodology, yet neither addresses the interface between DT operational data streams and SR metrics.

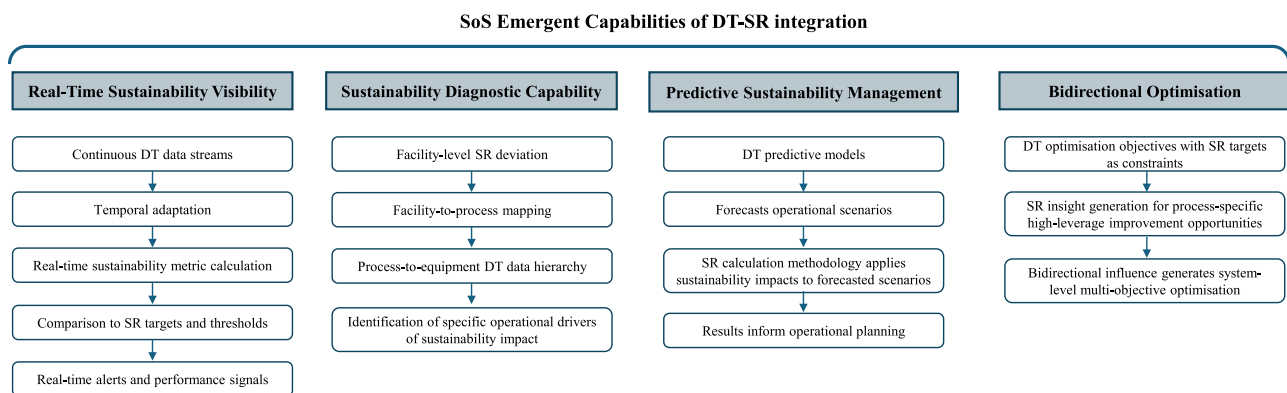


Figure 1. Theoretical mechanisms of SoS emergent capabilities: the DT-SR integration. Source: Authors' own work.

Table 3. Positioning of this study among Key DT, SR, and DT–SR studies.

Study	DTFocus	SRFocus	DT-SR Data Integration	System Boundary	Research Focus and Approach	Empirical Grounding
Ivanov (2024)	Y	N	N	System (SC network)	SC framework conceptualisation	N
Bhandal et al. (2022)	Y	N	N	System (operations and SC)	Bibliometric literature review	N
Liu, Zheng, and Bao (2024)	Y	N	N	Machine to System (single machine to manufacturing enterprise)	DT reference model development	N
Kumbhar, Ng, and Bandaru (2023)	Y	N	N	Process and Plant (production cell and facility)	Discrete-event simulation case study	Y (single firm)
Tao et al. (2022)	Y	N	N	Product (product design and lifecycle)	Data and model fusion framework	N
Badakhshan and Ball (2023)	Y	N	N	System (Inventory and cash management)	Simulation-optimisation modelling	N
Badakhshan and Ball (2024)	Y	N	N	System (SC planning)	Simulation-optimisation modelling	N
Osobajo et al. (2022)	N	Y	N	System (corporate sustainability reporting)	Bibliometric literature review	N
Silva, Nuzum, and Schaltegger (2019)	N	Y	N	System (corporate sustainability disclosure)	Systematic literature review (stakeholder theory applied)	N
Abeysekera (2022)	N	Y	N	System (corporate reporting framework)	SR conceptual framework (institutional theory applied)	N
Juvvala, Sangle, and Tiwari (2025)	Partial ^a	Y	N	System (logistics sector ESG performance)	ESG performance analysis with multi-firm survey	Y (multiple firms)
Kamble et al. (2022)	Y	Partial ^b	N	System (sustainable manufacturing SC)	Systematic literature review on DT for sustainable manufacturing	N
Li et al. (2020)	Y	Partial ^b	Partial ^c	Plant (single manufacturing facility)	Multi-criteria sustainability assessment	Y (single firm)
Tagliabue et al. (2021)	Y	Partial ^b	N	Plant (single educational building)	IoT and BIM sustainability assessment	Y (single plant)
Perotti et al. (2024)	Partial ^a	N	N	Plant (warehouse operations)	Technology review and conceptual development	N
This study	Y	Y	Y	Machine to Plant to System (nested, from operational process to corporate reporting boundary)	Conceptual framework development and illustration (System-of-Systems theory applied)	Y (evidence from seven firms)

Note: DT = Digital Twin; SR = Sustainability Reporting; Y = yes; N = no; SC = Supply Chain; IoT = Internet of Things; BIM = Building Information Modelling. System boundary labels follow the Scope and Scale dimension of Table 1.

^aDT referenced as enabling tool, not primary focus (Juvvala, Sangle, and Tiwari 2025); DT reviewed as one of multiple Industry 4.0 technologies (Perotti et al. 2024).

^bSustainability performance addressed without alignment to formal disclosure standards (Kamble et al. 2022); internal sustainability metrics only, no external reporting alignment (Li et al. 2020); building energy performance assessed without formal SR standards (Tagliabue et al. 2021).

^cInternal indicator weighting only, no mapping to disclosure standards (Li et al. 2020).

Table 3 maps and compares related studies across six dimensions, namely DT focus, SR focus, DT-SR data integration, system boundary, research focus and approach, and empirical grounding. Most DT studies operate at machine, process, or supply-chain scale without SR interface, while SR studies mainly address disclosure governance without operational data connections, reflecting a disciplinary divide in which these two bodies of literature have developed largely independently. Sustainability governance under mandatory reporting frameworks remains an unresolved priority in the current DT research agenda (Finco et al. 2026). The closest work bridging DT and SR, including Kamble et al. (2022), Li et al. (2020), Tagliabue et al. (2021), and Perotti et al. (2024), connects DT and sustainability performance in varying ways, though formal disclosure standard alignment (GRI, ESRS, ISSB), auditable data translation protocols, and SR governance design fall outside the scope of each. This study addresses these gaps through a structured four-step framework grounded in SoS theory. The confirmed research question is: ‘How could manufacturing digital twins (DTs) facilitate and enhance corporate sustainability reporting (SR)?’

3. Research design

3.1. Methodology

This research adopts a conceptual modelling approach supported by interviews to investigate the integration of reportable sustainability metrics with manufacturing DTs (see Figure 2). In the absence of research and practice, this necessarily exploratory study focuses on theoretical framework development and illustration, not empirical validation.

Literature review. First, the integration of sustainability within DT systems remains an emerging area, requiring a theoretical foundation to guide empirical inquiry and align research design, data collection, and analysis. As noted earlier, SoS theory offers a critical lens by conceptualising complex manufacturing systems as interdependent and nested subsystems with emergent properties (Maier 1998). This perspective helps explain how DTs, operating as autonomous yet interoperable entities, dynamically interact with SR to enable system-level performance monitoring. Building on this foundation, literature is used to develop a conceptual framework to capture data flows, metric aggregation, and reporting

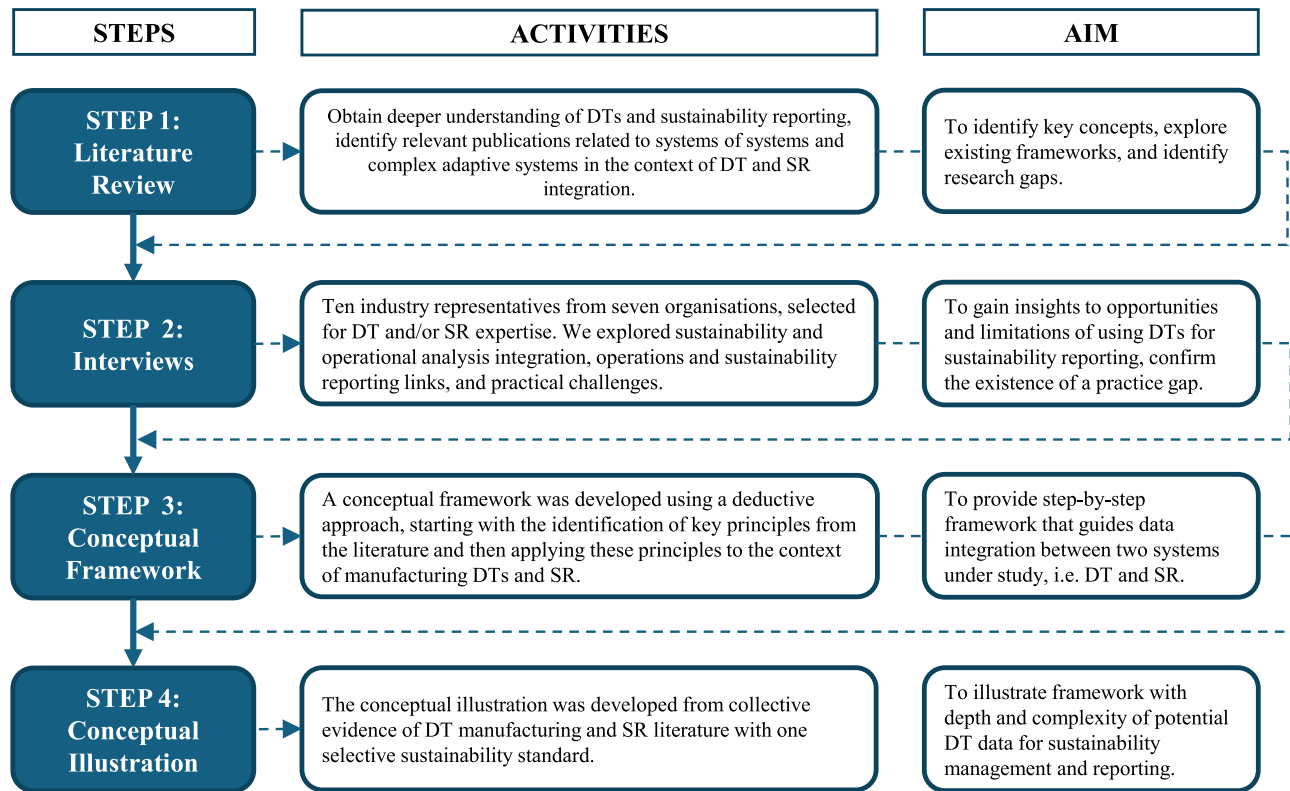


Figure 2. Research methodology. Source: Authors' own work.

Note: The research methodology follows the conceptual modelling approach of Robinson (2014) and Shannon (1998).

hierarchies across operational, facility, and corporate levels. It also facilitates the identification of research gaps, particularly regarding how DTs influence sustainability outcomes and how DT insights inform organisational decision-making.

Interviews were used as a qualitative data collection method to ensure contextual validity of DT-SR integration. The university ethics committee approved an application that demonstrated compliance with codes of practice, ethical guidelines on research integrity and the General Data Protection Regulation (in line with University Data Management Policy) of the university and the funder.

Ten participants from seven different companies were selected (Table 4). Purposeful sampling ensured inclusion of company representatives with relevant expertise and direct experience. The selection was not meant to be a representative sample of the UK but to provide insights from diverse experts in the field. The company selection criteria considered: a focus on sustainability or technology, the use of DTs within the business and the development of software for sustainability challenges. These criteria favoured the selection of cases 'most likely illuminate the research questions' (Yin 2014, 28). Semi-structured interviews used an interview protocol composed of 9 guiding questions (see Appendix 3).

The interviews with 'knowledgeable agents' (Gioia, Corley, and Hamilton 2013) typically lasted 60 min and were conducted online via the Zoom platform. The interviewees were high-level managers or senior executives to address the strategic nature of the questions contained in the interview protocol. The company names were anonymized (use of code A to G) with a generic description for each. The same applied to individual participants by using their job titles and not their names.

For data processing and analysis, three main steps were followed: data transcription, data organisation, and open coding. First, the interview recordings were transcribed to enable thematic analysis. The initial transcription used the automated transcription function on the Zoom platform. These transcripts were subsequently manually corrected, reviewed and organised in tables to enable comparison of question-responses across interviewees. This systematic organisation of the qualitative data supported the identification of patterns and relationships within the dataset. Finally, the data were analysed through open coding, whereby the material was broken down into analytical categories to support interpretation of the phenomenon under study. These coding categories were developed through iterative, interpretative, and reflexive reading of the transcripts.

Table 4. Profiles of the companies and interviewees.

Company	Description	Size	Interviewees	Role in the Company	System Expertise*
Company A	Consultancy: sustainability strategy	Small	1	• Director	2
Company B	Consultancy & software provider: simulation, optimisation, data science	Large	3	• Simulation expert • Business development lead • Sustainability expert • Sustainability lead	1,2
Company C	Consultancy: digital transformation solutions (sustainability)	Medium	2	• Managing consultant	1
Company D	Consultancy & software provider: simulation, optimisation, data science	Small	1	• Chief technology officer	1
Company E	Consultancy: – digital transformation solutions (general)	Large	1	• Client innovation lead	1, 2
Company F	Manufacturer: automotive	Large	1	• Sustainability director (former)	1
Company G	Manufacturer: aerospace	Large	1	• Industrial eco-designer	1, 2

Note: All company names are anonymized using codes A to G. Individual participants are identified by job title only. System 1: manufacturing digital twins; System 2: sustainability reporting, consistent with the two subsystems defined in Sections 2.2 and 2.3.

Source: Authors' own work.

The conceptual framework was developed deductively. Principles derived from literature and refined by interviews were systematically applied to the manufacturing context. Conceptual modelling techniques were employed to visualise components and relationships in a framework as nested, hierarchical structures. Such techniques refer to the abstraction and formalisation of a real system into a structured abstract representation that captures its key elements, relationships, assumptions, and intended behaviours prior to empirical modelling (Robinson 2014; Shannon 1998). This is appropriate where empirical data are scarce, fragmented, or not yet fully developed. Such scientific reasoning processes provide theoretical clarity, define the scope of the system under study, and identify the mechanisms through which subsystems (e.g. DT and SR) interact to yield emergent system-level behaviour. A conceptual framework comprises the problem definition, system boundary specification, identification of key entities and relationships, assumption articulation, model representation and visualisation, and conceptual validation (Pidd 2014).

The conceptual illustration of DT and SR potential was developed from manufacturing and sustainability reporting literature, the selected sustainability standard, and interview informed application examples.

3.2. Interview results – interconnected systems

This section brings together interview insights with literature to support the development of a framework for manufacturing systems and sustainability reporting systems interconnection. Interviews revealed two major challenges in the integration of DTs (System 1) with SR (System 2): data integration and the difficulty of shifting from data to strategic decision-making (see example quotes from interviews in Appendix 4).

3.2.1. Data integration

Interviewees cited the fundamental challenge to integrate DTs with SR lay in the mismatch between data types and reporting requirements. DTs operate with high-frequency, granular data, while sustainability reporting relies on aggregated, periodic data, e.g. annual or quarterly reports. This discrepancy complicates the direct use of DT-generated insights for sustainability performance enhancement. While DTs can support sustainability reporting by consolidating operational data, organisations often face technical barriers such as data availability, inconsistent collection methods, and incomplete sensor deployment. This explains and confirms the manufacturing and reporting data divide uncovered in the literature review. Despite this, companies still obtain the data for reporting.

Interviewees asserted certain sustainability indicators, such as carbon footprint, require integration of multiple data sources, e.g. energy, materials, waste, transportation. While DTs could support metrics related to climate change, pollution, and water use, areas like biodiversity and circular economy present greater challenges due to lack of standardised measurement frameworks and cross-organisational dependencies. Further they emphasised that overcoming these hurdles necessitates mapping DT outputs to sustainability reporting inputs, using standard processes that ensure DT-generated insights support decision-making. This reinforces the incompatibility present in literature.

3.2.2. From data to decision-making: moving beyond efficiency toward strategic sustainability

The second challenge revealed by interviewees lies in how DTs are used in decision-making. Manufacturing DTs focus on efficiency, risk management, and cost reduction, with limited consideration of sustainability-driven decision-making. Prioritisation is given to financial incentives over sustainability goals, meaning DTs are

primarily deployed to avoid risks and optimise investments rather than to support sustainability reporting or strategic environmental improvements. This suggests a motivational reason for the current divide between manufacturing DTs and SR systems covered in the literature review rather than a lack of value of integration.

From the interviews, the potential of DTs to optimise processes for sustainability in real-time was evident. Emerging DT applications, such as in the pharmaceutical and fashion industries, were cited that align production schedules with energy availability, quantify CO₂ reductions, and support sustainability trade-offs. These isolated cases lack frameworks to integrate DT-generated data into sustainability metrics. Interviewees stated that even if data is available, organisations often lack the internal capacity to interpret sustainability trade-offs effectively, e.g. balancing carbon emissions with waste reduction. While literature is sparse, emerging applications taking a more systematic approach were cited by interviewees.

The interviewees saw that the absence of frameworks was a barrier for linking DT data to sustainability performance indicators, making it difficult to integrate these insights into corporate strategy and decision-making. Additionally, it was apparent from them that expanding DTs beyond operational sites to value chain-wide sustainability management introduces legal, technical, and organisational challenges, such as data confidentiality, inconsistent formats, and unwillingness to share information across organisations. We can conclude that frameworks are absent in both theory and practice.

Overcoming these barriers requires the development of integrated frameworks, AI-enhanced scenario modelling, and improved workforce capabilities to embed sustainability considerations into data-driven decision-making.

4. A system-of-systems DT-SR integration framework

4.1. Establishing systems relationships

This study focuses on the manufacturing enterprise. Any DT exists within the boundary of the manufacturing system. It views DTs and SR as distinct yet interacting systems within the manufacturing enterprise. The framework is principally designed to operationalise environmental sustainability metrics (energy, emissions, and resource flows), which correspond most directly to quantitative DT outputs; social and governance metrics are considered where they are digitally traceable within the manufacturing system boundary. Using SoS theory and

conceptual modelling, key components in nested subsystems and data flows are identified and their interrelationships explored. Figure 3 illustrates the generic input-and-output data flow between Manufacturing DTs (System 1) and SR (System 2), showing their mirrored relationship. The data exchanges illustrate the SoS interface, where emergent capabilities are generated and identified in Section 2.6 and detailed in Figure 1.

The DT-SR integration framework (Figure 4) builds on the SoS data flows (Figure 3). The framework shows the mapping of data flows between two systems, demonstrating how a DT and SR interact to offer emergent capabilities. This integration allows evolutionary development while maintaining operational independence of both systems. The integration is iterative; as manufacturing processes and reporting standards evolve, interfaces adapt without disrupting core systems. Bidirectional (not unidirectional) data flows enable the operational system to provide data for the reporting system for sustainability targets to in turn guide the manufacturing decisions, offering system-level sustainability optimisation.

4.2. Operationalising the framework

Here we expand on the conceptual framework to show the step-by-step operationalisation process (Figure 5) that integrates DT and SR data in manufacturing. The framework incorporates a four-step process – mapping, matching, measuring, and modelling – aligning granular DT input-output data with sustainability metrics. Due to differences in scale and purpose, exact matches are not always possible, requiring intermediary conversions or additional inputs. Rooted in conceptual modelling, the framework translates abstract models into a visual representation of DT and SR interrelationships. Diagrammatic visualisation clarifies how DT-generated operational data is systematically mapped into sustainability metrics.

4.2.1. Step 1: mapping

This step identifies relevant sustainability and DT data within manufacturing, laying the foundation for data matching, measuring, and modelling. Four checkpoints guide this process:

Checkpoint 1.1 Review of sustainability disclosure standards: Requirements are analysed to identify key reporting categories and metrics, forming a baseline for DT comparison and revealing data gaps.

Checkpoint 1.2 Inventory of sustainability-related information: Existing data is assessed, recognising that sources may be fragmented. Data, like water consumption, may

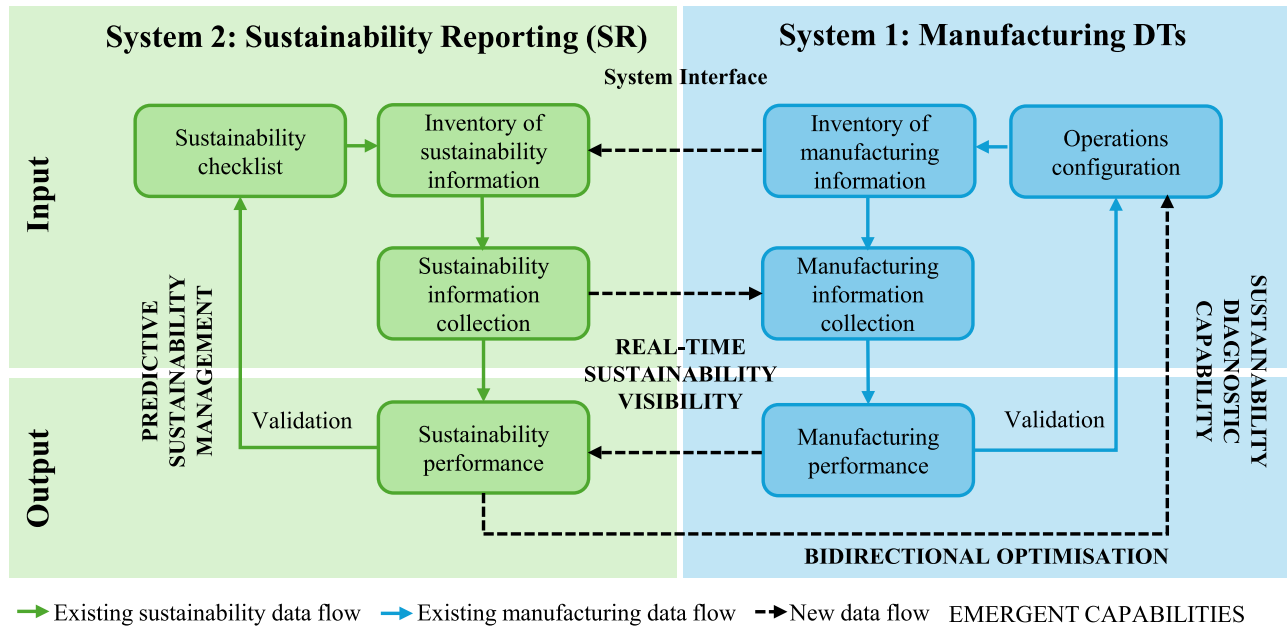


Figure 3. System-of-systems overview of data flow between manufacturing DTs and SR. Source: Authors' own work.

Note: The data flow is structured from the data requirements of SR (System 2) on the left to the data supply capability of DTs (System 1) on the right, reflecting the mapping logic of Step 1 in the framework. System 1 = manufacturing digital twins (Section 2.2); System 2 = sustainability reporting (Section 2.3).

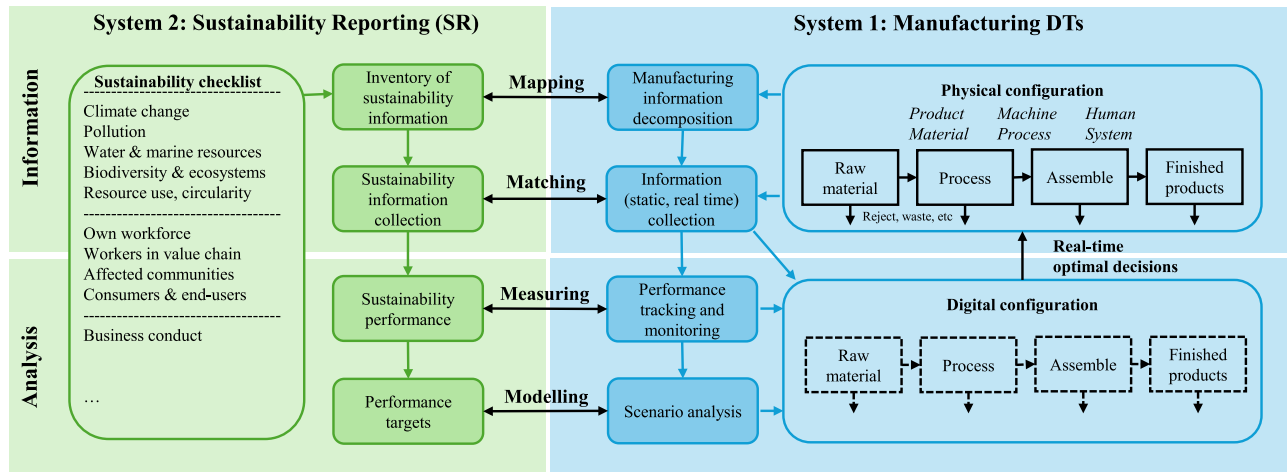


Figure 4. A DT-SR integration framework: synergies between manufacturing DTs and SR. Source: Authors' own work.

Note: The integration framework builds on Figure 3 by showing the bidirectional data exchange between System 1 and System 2, where DT operational data informs SR outputs and SR targets feed back into DT-enabled operational decisions. System 1 = manufacturing digital twins (Section 2.2); System 2 = sustainability reporting (Section 2.3).

require allocation across activities if unavailable at a granular level.

Checkpoint 1.3 Initial mapping of data sources: Sustainability metrics are linked to available data sources, pinpointing areas where DTs can bridge gaps, including sensors, IoT devices, databases, and historical records.

Checkpoint 1.4 Pooling of data flows: Aggregation across multiple production sources (e.g. multiple machines) prepares for the next step, namely data matching.

4.2.2. Step 2: matching

SR data must align with that from the DT. This step defines the data matching process to guide assessments and potential automation and establishes measurement formulae for each sustainability metric.

Checkpoint 2.1 Direct linkages: DT data matches with sustainability metrics are identified.

Checkpoint 2.2 Indirect linkages: Relationships are mapped via transformations (e.g. converting material

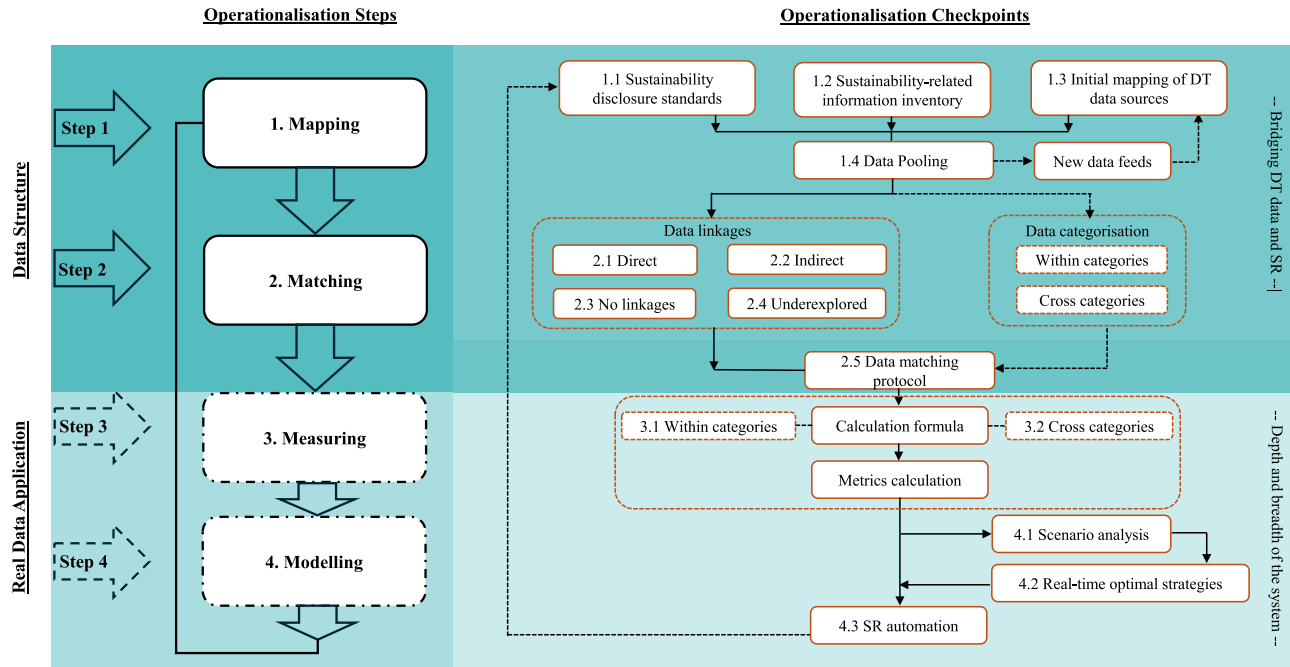


Figure 5. A step-by-step operationalisation approach for the DT-SR integration framework incorporating checkpoints. Source: Authors' own work.

Note: Checkpoint numbering follows the four-step operationalisation process defined in Section 4.2.

handling into CO₂ emissions) and documented for integration and potential refinement.

Checkpoint 2.3 No linkages: Unmatched DT data is recorded as gaps, clarifying irrelevant elements for SR while retaining them for broader model execution.

Checkpoint 2.4 Underexplored linkages: Some sustainability metrics highlight missing DT data, prompting additional data collection or system updates to meet evolving sustainability needs.

Checkpoint 2.5 A standardised data-matching protocol: Procedures are established for further integration. For instance, machine energy data supports SR metrics on efficiency and equipment lifespan.

4.2.3. Step 3: measuring

With data aligned, metrics are calculated based on relationships established in Step 2.

Checkpoint 3.1 Direct calculations within categories: Some metrics are computed by aggregating data within a category, e.g. summing machine energy consumption to determine total energy use.

Checkpoint 3.2 Combining data across categories: More complex metrics require data combinations, e.g. carbon footprint calculations integrating energy, material use, and waste data. Standardised formulas ensure consistency.

4.2.4. Step 4: modelling

Calculations from Step 3 are used to assess sustainability performance and identify improvement opportunities.

Checkpoint 4.1 Scenario analysis: Examines how changes impact SR metrics. Here strategic options for optimising resource use, waste reduction, and production efficiency are explored. For example, production schedules may be adjusted in response to anticipated demand fluctuations or machine availability, with the objective of aligning operational practices more closely with SR targets.

Checkpoint 4.2 Real-time optimal scenario analysis: At this stage, the DT system functions as a structured repository, offering data-driven insights for comparisons with SR targets. This step prepares for future goals around predictive analytical capabilities.

Checkpoint 4.3 SR automation: Future advances, not considered in this research, could embed intelligence for real-time responses. Automated data mapping, calculation formulas, and scenario modelling could enhance decision-making, ensuring sustainability metrics remain adaptive to changing regulations and technologies.

5. Framework application: a conceptual proof of concept

5.1. A generic manufacturing model

The step-by-step integration framework in Figure 5 outlines how DT data can connect with system-level sustainability metrics. To illustrate the framework's potential, a generic production system is used as proof-of-concept. To sufficiently reflect reality, the conceptual static illustration includes multiple production stages using data types from literature. Future research could validate a more complex, dynamic case.

Figure 6 visualises the DT manufacturing parameters, including data flow and scale. Following Kumbhar, Ng, and Bandaru (2023), three key processes are included: (A) machining (milling and turning), (B) assembly, and (C) quality assurance. Supporting operations involve material handling using automated guided vehicles (AGVs), robots, and operators. The data flows depicted in Figures 4 and 6 are used to make the DT-to-SR data transformation logic explicit. Figure 4 illustrates the integration framework at the system level, while Figure 6 shows the DT data categories and flows at the manufacturing unit level. Together, they provide a visual representation of how operational data is structured for downstream transformation into standardised SR metrics.

The primary category for the input and output data is identified (scale). This constitutes the preliminary mapping informed by relevant literature including Liu, Zhou, and Tang (2020) and Morgan and O'Donnell (2017) for

CNC machining twins; Li et al. (2023) and Chen et al. (2015) for assembly twins; Liu et al. (2021) for quality assurance; and Sharotry et al. (2020), Lin et al. (2024), Montini et al. (2021), and Yang et al. (2024) for operators. This paper focuses on internal manufacturing processes and leaves external connections for future research given that data integration across all factories and supply chain members cannot be underestimated (Tufano 2023). Next steps 1–4 of mapping, matching, measuring and modelling are carried out.

5.1.1. Step 1: mapping

Checkpoint 1.1 Review of sustainability disclosure standards: Here ESRS is used as the chosen mandatory EU standard. The sustainability checklist provides a baseline for DT comparison, identifying data gaps.

Checkpoint 1.2 Inventory of sustainability-related information: the three core dimensions (environment, social, and governance) with 10 topics (e.g. climate change, pollution, biodiversity, circular economy, workers, communities, business conduct) and 40 sub-topics (e.g. climate adaptation, pollution of water, working conditions, corporate culture) are utilised. Appendix 2 exemplifies ESRS E1 (Climate Change).

Checkpoint 1.3 Initial mapping of data sources: The extensive inventory data – including machine sensors; IoT devices on assembly lines, robots, and AGVs; databases for materials and product storage; and historical records on machining, assembly, and quality rejection rates – are sourced. Data sources may be fragmented across scales, such as energy consumption by machines, lighting and HVAC (Heating Ventilation and

CATEGORY	MACHINING OPERATIONS	ASSEMBLY OPERATIONS	QUALITY PROCESSES	STAFF
Example	CNC machine	Assembly station	Quality checks	Machine operators
Process INPUTS	- Geometry - Machine setting - Machining procedure - Parameters - Operators - Energy	- Bills of Materials (BOM) - Orders - Geometry - Physics - Machining sequence - Parameters - Tolerance - Operators - Energy	- Operators - Process - Fixture - Material - Machine/Tool - Inspection procedures - Environmental info	- Body kinematics - Social interaction - Behaviour - Physiologies - Biometrics - Environmental info - Physical activities - Range of motion (ROM)
Process OUTPUTS	- Material waste - Envelope surface - Machining cycle - Tool/Machine state - Success rate	- Assembly cycle - Product fixture - Tool/Machine state - Success rate	- Product quality - Process quality - Success rate	- Task execution time - Task execution accuracy
DT OUTPUTS	- Energy consumption - Material utilisation - Material waste - Operator working hours - Machine fatigue analysis	- Assembly quality - Geometric deviation - Error propagation	- Process quality evaluation - Product quality evaluation - Outsourcing parts quality evaluation	- Operator fatigue - Bio feedback on motion - Centric statistics - Mental stress
Sources	Liu et al. (2020) Morgan and O'Donnell (2017)	Li et al. (2023) Chen et al. (2015)	Liu et al. (2021)	Sharotry et al. (2020) Lin et al. (2024) Montini et al. (2021) Yang et al. (2024)

Figure 6. A DT model of a simple manufacturing unit illustrating data flow by scope and scale. Source: Authors' own work.

Note: Scope and scale dimensions follow the data categories defined in Table 1.

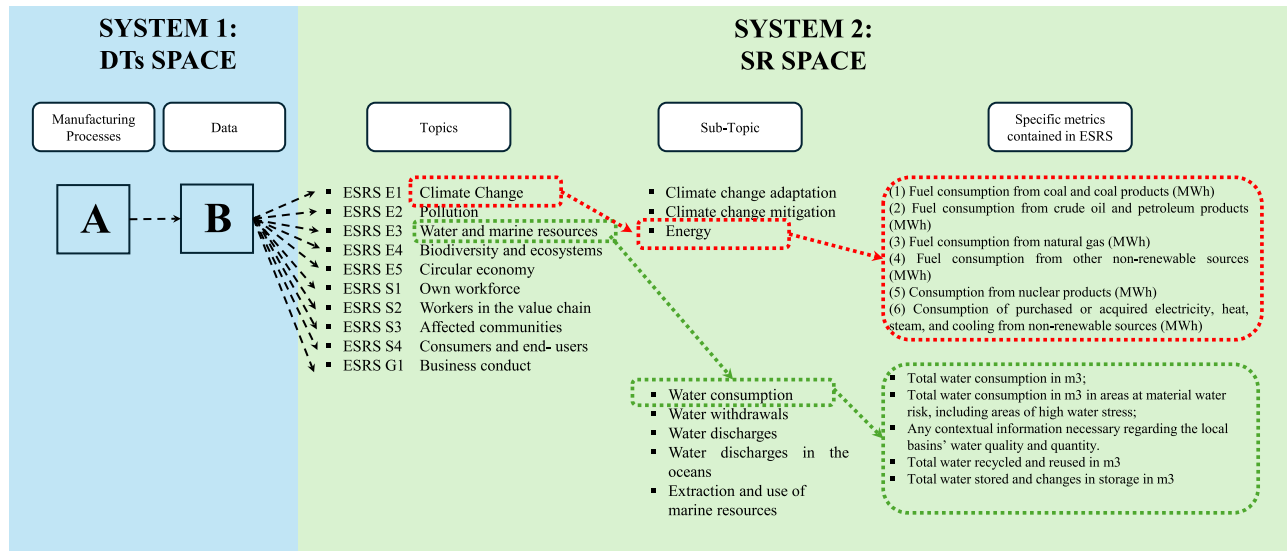


Figure 7. Matching process between manufacturing DT data and ESRS metrics. Source: Authors' own work.

Note: ESRS = European Sustainability Reporting Standards. Matching logic follows the data-matching protocol established in Section 5.3.

Air Conditioning). Machine data can be tracked directly, while facility energy consumption must be allocated specific production areas. Allocation decisions are documented as they impact the effectiveness of sustainability reporting. DTs typically produce data at high operational frequencies (e.g. per production cycle or in near real-time), whereas SR frameworks require aggregated data over fixed reporting intervals (e.g. monthly, quarterly, or annual). The interval for each metric is defined alongside the aggregation logic to form an audit trail. Where sensors are absent or provide incomplete data, the approach to handling missing values such as last-known-value substitution, interpolation, or explicit gap-flagging, is also logged.

Checkpoint 1.4 Pooling of data flows: here data collection and aggregation are prepared for Step 2: Matching. For example, energy consumption over time for machines, assembly lines, AGVs, robots, lighting, HVAC, IT systems, and sensors. This allows for effective matching later on by analysing the contribution of each source.

5.1.2. Step 2: matching

From the preliminary mapping, we have an inventory of DT data available and sustainability data aligned to the standard. Next the information is matched.

Checkpoint 2.1 Direct linkages: The identification between DT data and sustainability metrics is illustrated in Figure 7 where each input-output element within manufacturing processes (A) and specific data points (B) are mapped directly to sustainability topics, subtopics, and specific metrics. For example, ESRS E1 (climate change – fuel consumption) and ESRS E3 (water consumption) are paired to machine energy or process water data.

The sustainability data scale and scope dimensions are given by the standard (i.e. topics, subtopics, metrics) and aligned with the input-output data in the manufacturing DTs, essentially matching metrics sharing the same data attribute.

For example, under ‘material handling by human operators’ there are ‘physical activity intensity level’ (input data) and ‘operator centric statistics’ such as worker scheduling and rest interval (output data) which relate to ESRS S1, Own Workforce working conditions, e.g. secure employment. The same may apply to ‘human-environmental data’ (temperature, humidity, cleanliness, illumination, etc.) and ‘human-human social interaction data’, that may be associated with mental stress. Aligning energy consumption (for ESRS E1) is straightforward for many manufacturing processes, perhaps explaining why this is dominant in literature.

Checkpoint 2.2 Indirect linkages: These are more complex to measure or simply non-existent. The challenge is aligning data, re-composing and calculating. Sustainability data with less evident or missing links to DTs (i.e. materials or removed materials) are ESRS E2, E3 and E4, related to pollution, water and marine resources and biodiversity, respectively. For the assembly process, the BOM can indirectly relate activities to pollution (materials type, origin, toxicity, etc.). Lastly, ESRS E5 circular economy may be easier for firms with developed circular business models well beyond recycling, removed materials, rejected components and rejected products, documented or calculated from the bill of materials. Where indirect linkages require data transformation, for instance, converting material handling energy into Scope 1 or 2 GHG

equivalents using standard emission factors, or applying waste characterisation data to derive pollution load estimates, the conversion methodology, factor source, and version are recorded in the data-matching protocol. This documentation forms the basis for provenance logging and supports subsequent audit and verification of reported sustainability metrics.

Checkpoint 2.3 No linkages: DT data lacking relevance to sustainability requirements and able to be excluded from further analysis (or flagged for future applications). Examples include geometry, physics and surface.

Checkpoint 2.4 Underexplored linkages: This checkpoint seeks to identify opportunities not considered previously. For example, if an alteration in machining sequence could enhance sustainability performance or if waste materials offer circularity opportunities. Other opportunities could include maintenance, air quality, operator behaviour and social interaction, work health, etc. It may be necessary to collect new data.

Checkpoint 2.5 A standardised data-matching protocol: The last checkpoint unifies data-matching procedures across manufacturing, e.g. asset sensor readings, factory energy consumption, indoor air quality, staff physical activity intensity, etc.

5.1.3. Step 3: measuring

This chain makes explicit how Step 2 matching protocols govern Step 3 calculation inputs, and how the provenance log supports audit. Figure 8 illustrates the data aggregation flow used to measure sustainability indices in manufacturing, as operationalised in Step 3 of the framework. The figure shows how prepared and categorised data from DT systems are applied to SR metric calculations. The figure delineates how granular DT data points are assigned to specific metrics based on prior data mapping and matching. These data are then aggregated at the sub-topic level and consolidated into broader topic-level indicators within the ESRS framework. The visualisation reflects both straightforward calculations such as summing machine-level energy data, and more complex aggregations where multiple data categories must be integrated.

Checkpoint 3.1 Direct calculations within categories: An illustrative example from Figure 8 is the ESRS E1 climate change, specifically energy consumption. Consider a CNC machining cell operating one eight-hour shift. Measured electricity consumption across three machines totals 240 kWh (aggregated via Checkpoint 1.4); a 15% facility overhead allocation for HVAC and lighting adds 36 kWh, giving 276 kWh for the shift. Applying the UK national grid Scope 2 emission factor (0.233 kgCO₂e/kWh, DESNZ 2024) yields 64.3 kgCO₂e.

Annualised and aggregated across all facility sub-units, this produces the ESRS E1 disclosure figure in tCO₂e.

Checkpoint 3.2 Combining data across categories: The second illustrative example from Figure 8 is the ESRS S1 workforce. Here operator activity is summed per shift and normalised per full-time equivalent.

5.1.4. Step 4: modelling

Step 4 focuses on the application of the previously developed sustainability performance calculations (from Step 3) to simulate and evaluate operational scenarios within the DT-supported manufacturing system. This stage represents the transition from descriptive measurement to prescriptive modelling, enabling firms to explore the cause-effect relationships between operational changes and sustainability performance metrics through structured scenario experimentation. The modelling process includes scenario analysis (Checkpoint 4.1), real-time optimisation (4.2), and SR automation (4.3), dynamically configured using DT data. It follows standard simulation procedures, including problem definition, model construction, validation, and experimentation (Law 2007; Robinson 2014).

Checkpoint 4.1 Scenario analysis: Interviewees emphasised the necessity for scenario-based analyses that reflect real-world operational challenges and strategic sustainability priorities. Accordingly, this checkpoint is grounded in practitioner evidence. Each scenario below is drawn from interview testimony of implementation work by their organisation or work by them for a client organisation. Five scenarios are presented to illustrate how DT-generated operational data can be modelled against four sustainability dimensions, namely energy-aware scheduling, social metric capture, circular economy tracking, and supply chain integration. Together, they confirm that while industry is pursuing sustainability monitoring using DT data and modelling capabilities, the scope of the DT-SR framework is only partially implemented in practice. Practitioner quotes are used to support each scenario.

Scenario (a) – waste reduction and energy optimisation: Company D is developing production monitoring to reduce waste and improve energy efficiency while maintaining throughput targets. Modelling evaluates process efficiency and energy mix configurations under different operational constraints. This would impact on ESRS E1 Climate change (energy intensity and carbon) and E5 Resource use and circular economy (waste generated and reused).

In terms of the question about sustainability, many of the models we have been working on focussed on not just from the capacity point of view, i.e. how do we balance the level of production that is required, but also with

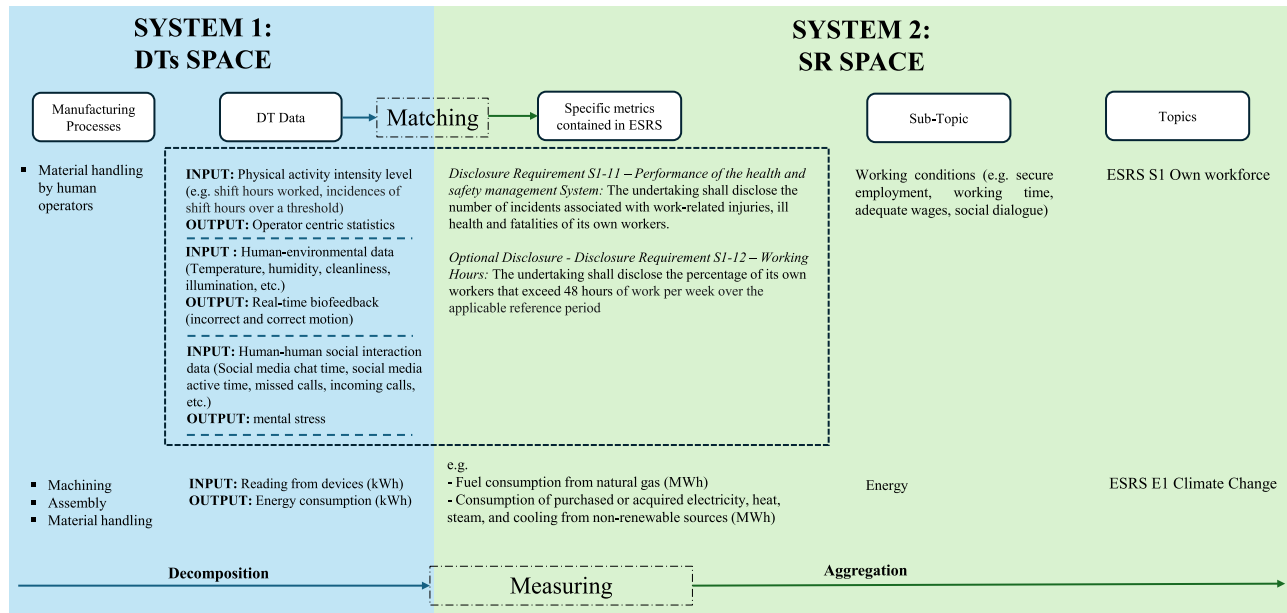


Figure 8. Example of data flow for measuring sustainability indices. Source: Authors' own work.

Note: The data flow runs from left to right, from granular DT data inputs aggregated via Steps 1 and 2 through to calculated sustainability indices at topic and sub-topic level under ESRS. Direct calculations (Checkpoint 3.1) aggregate data within a single category; cross-category calculations (Checkpoint 3.2) combine data across multiple sources. ESRS = European Sustainability Reporting Standards; E1 = Climate Change; S1 = Own Workforce.

the increasing sustainability requirements that have been set, from compulsory point of view. That included measuring the amount of waste produced within the system and minimising that, as well as making the processes as efficient as possible. Also considered the energy aspect (energy mix between renewables and energy pull from the grid). But it does require the actual data pipeline, the detail of that data (granularity) to work consistently with the production system – Chief Technology Officer, Company D.

Company D demonstrates the data pipeline logic underpinning Steps 1 to 3, where granular production data on waste and energy mix feeds directly into sustainability calculations, confirming the Measuring step's dependency on consistent and detailed data flows.

Scenario (b) – energy-aware batch scheduling: Company C optimises batch production in high-energy sectors (the case of pharmaceuticals) by integrating real-time energy data to schedule production when renewable energy availability is highest, reducing carbon emissions. Impacts within the Sustainability Reporting (SR) would be concentrated on ESRS E1 Climate change (the proportion of energy coming from the different non-renewable fuel sources). Potentially indirectly this would impact on E2 Pollution though not reportable at company level.

In the pharmaceutical industry, companies are embedding the sustainability angle in the DT for the manufacturing of their products, e.g. specific drugs, for example when looking into energy aspects. Running a mathematical optimization, suggesting when the greenest times to produce the next batch of a given medicine, were based

on how much wind was blowing (as they were using a combination of solar and wind turbines as a source of renewable energy). It is the utility company that provides the data – Sustainability Lead, Company C.

Company C's pharmaceutical example represents the most complete instance of Checkpoint 4.1 scenario analysis, with a live mathematical optimisation keyed to renewable energy availability directly informing batch production scheduling. This is a direct instantiation of the DT-to-SR feedback loop, where operational decisions are shaped by sustainability targets.

Scenario (c) – social sustainability monitoring: Company F integrates operator well-being data into production planning, aligning workforce health metrics with SR objectives. This would impact on ESRS S1 (own workforce) in conditions around ensuring safe and healthy work environment, and work-life balance. This impacts on health and safety, mental health, and may inform labour standards and ergonomic improvements.

... for example, in a factory environment, one of the things that is often a well-being issue for the workers is what is the ambient temperature that they're actually working in. So, for example, if we say that the ideal temperature is 19 degrees centigrade on the shop floor, actually we could measure and characterize that by saying, well, for 98% of the year, we were 19 degrees plus or minus one degree, and therefore we contributed to the members well-being on the basis that we kept one of the known factors for their discomfort actually available and we can measure this now and we can give you a result – Former Sustainability Director, Company F.

Company F's temperature monitoring illustrates how SR social metrics under ESRS S1 can be generated from continuously measured DT data with quantified targets, demonstrating that workforce well-being indicators are technically tractable within the framework's Measuring and Modelling steps.

Scenario (d) – circular economy and material efficiency: A luxury fashion brand project (described by Company C) illustrates circular economy integration and track waste streams, integrating them with SR systems to improve circular economy reporting. This would impact ESRS E5 Resource use and circular economy indicators, and indirectly E1 and E2 with data supporting measures like recycling rates, material input ratios, and waste reduction metrics.

I mentioned a project we did last year with a luxury fashion brand and the kick-starter for the project was that they were looking at the eco-design for sustainable product regulation ESPR and within that one of the key requirements is that in order for them to sell their goods on the EU market, they need to produce a digital product passport for all of their products... that's a real challenge for them and effectively creates a digital twin for a t-shirt and they will be able to track that all the way from the top of the supply chain through to the point of sale, and there's also some technology partners that we interviewed as part of that project that are looking at creating platforms that can track the customer journey beyond the point of sale, to look at things like where are the points of resale, where are the points of repair and tracking that sort of circular customer journey with the idea that if they can capture that data and better understand customer behaviours post point of sale, that can maybe intervene and make sure that the life cycle of those products is extended or they're guided into resale rather than disposal – Sustainability Lead Company C.

Company A's circular economy project shows how DT data tracking material flows and waste streams can be connected to ESRS E5 reporting obligations, with the digital product passport approach offering a concrete model for provenance-based SR at the product level.

Scenario (e) – supply chain sustainability integration: Company B is extending its DTs beyond factory walls, working to extend DT boundaries beyond the factory to capture supplier data and transportation metrics into SR dashboards. Here the broader impact would most be around measuring Scope 3 emissions, ESRS E1 (Scope 3 GHG emissions), reporting on supply chain workers' conditions (ESRS S2), and tracking compliance with environmental standards across suppliers (ESRS G1).

If we're talking about the full sustainability area, it's getting that view into the supply chain. And that could be for CO₂, it could be for energy or whatever. But certainly for things like knowing the provenance of your materials from a you know... a social perspective. Where are you

getting your Cobalt from? Is it coming from some smelter in the Democratic Republic of Congo which is using artisanal mining, which is therefore using kids mining or the welfare of those people is not so good, it's very difficult to do that. There's various people that are working on it. Probably the most obvious one is to understand where your supply chain is coming from at the moment – Former Sustainability Director, Company F.

Company B's supply chain integration attempt illustrates the most expansive application of the framework, extending DT boundaries beyond the factory to capture Scope 3 emissions and supplier conditions under ESRS E1, S2, and G1, while also surfacing the legal and organisational barriers that make this the most challenging dimension to systematize.

Checkpoint 4.2 Real-time optimal scenario analysis: This checkpoint is covered within descriptions of the above scenarios.

Checkpoint 4.3 SR automation: Not considered in this research, however, this could embed intelligence for real-time responses.

Together, the five scenarios presented in *Checkpoint 4.1* reflect real industrial attempts at DT-enabled SR across the sustainability dimensions identified in this framework. None of these practices constitutes a full end-to-end validation of the four-step framework, as that remains the objective of the pilot design. What the evidence does establish is that each of the framework's constituent steps reflects active industrial concerns, and that practitioners have independently arrived at the same data connections the framework systematizes.

5.2. Future research

These scenarios presented demonstrate the framework's practical utility across diverse manufacturing contexts, reinforcing the DT's potential as a strategic tool for sustainability management. Together, they validate the four-step framework's operational capability to translate granular DT data into actionable SR metrics across the ESRS landscape. Further, the integration of DT outputs with SR requirements is expected to create operational efficiencies through data reuse, reduced redundancy in reporting, and enhanced decision-support capabilities. Figure 9 provides an overview of future research directions.

6. Discussion

This study addresses a literature gap regarding the application of manufacturing DTs in SR. Previous research acknowledges DTs potential for manufacturing operations optimisation (Mantravadi and Møller 2019; Shojaeinasab et al. 2022; Tagliabue et al. 2021) but leaves their role in corporate sustainability largely unexplored.

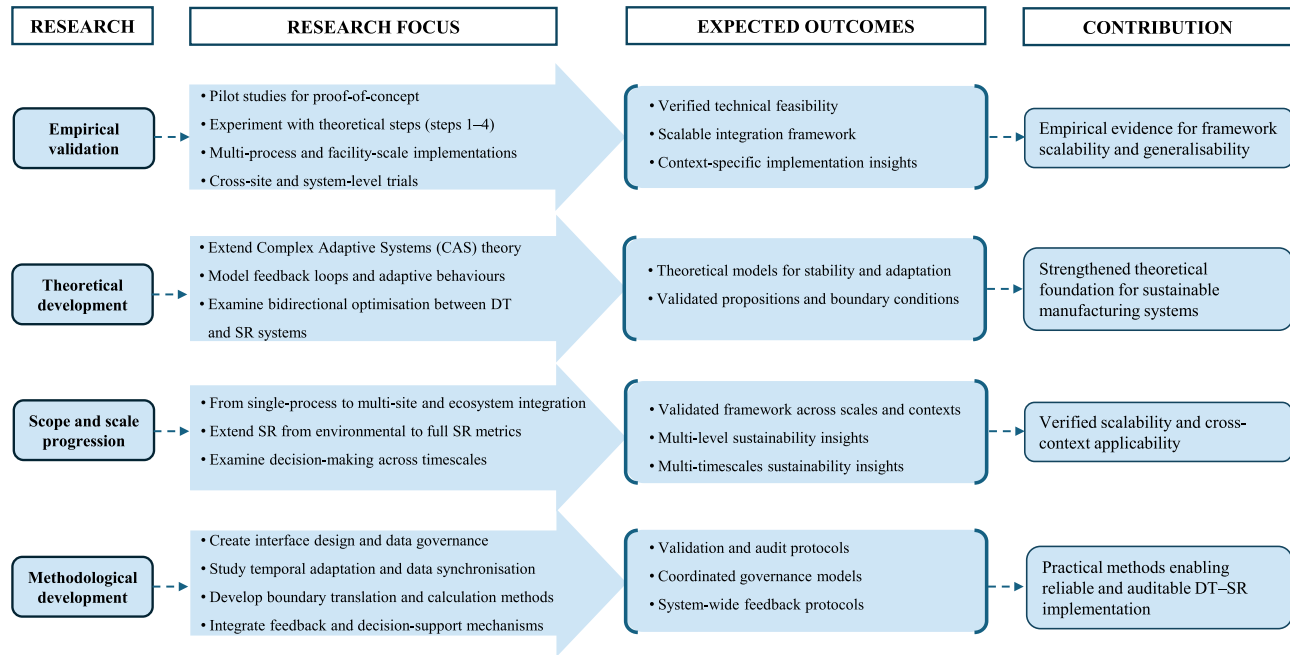


Figure 9. Future research directions for DT-SR integration. Source: Authors' own work.

Note: The future research directions are organised across four themes, namely empirical validation, theoretical development, scope and scale progression, and interface design and data governance, each mapped to its intended contribution to DT-SR integration knowledge. Arrows indicate the recommended sequence of research progression, with empirical validation as the foundational first step. Source: Authors' own work.

Our findings extend the literature by demonstrating how manufacturing systems can be systematically aligned with sustainability systems through DTs, with potential for adaptive responses and enhancing both SR and strategic decision-making. This contribution is relevant to the growing field of sustainable manufacturing practices, extending DTs as a critical tool for dynamic reporting that responds to dynamic operational data (Tagliabue et al. 2021).

While SoS defines the architecture and interfaces, the dynamic and adaptive behaviour of the integrated DT-SR system (i.e. bidirectional optimisation) reflect the fundamental properties of Complex Adaptive Systems (CAS) theory. From the CAS perspective, DTs are not static models but are dynamic entities that adapt as new data are acquired from the physical system (Nair and Reed-Tsochas 2019; Surana et al. 2005). Such adaptability enables a responsive and forward-looking manufacturing system to mitigate risks, optimise sustainability performance, and enhance resilience. For instance, Juvvala, Sangle, and Tiwari (2025) discuss how sustainability-driven DT implementations enable logistics firms to adjust operations dynamically based on sustainability performance metrics, illustrating a self-organising mechanism characteristic of CAS. Similarly, Messina, Eslami, and Castilla (2025) emphasise how blockchain-enhanced DTs support decentralised and adaptive governance models, demonstrating distributed

intelligence for responsiveness. Niu, Zhang, and Dong (2025) demonstrate a related self-organising mechanism, using blockchain-based multi-tier product tracking to mitigate data inconsistencies across supply chain tiers with real-data validation. The adaptive and iterative characteristics of the proposed DT-SR framework warrant further exploration from the CAS perspective, particularly in the design of system interfaces that enable seamless bidirectional feedback and learning within the integration process.

Although certain sustainability indices can be calculated from manufacturing data, aggregating data across multiple scales to produce comprehensive system-level sustainability reports remains a substantial challenge. The findings demonstrate how a conceptual modelling and simulation mindset can facilitate this transformation.

The framework application illustrates how a DT could rigorously address SR requirements in a simplified manufacturing system. More extensive automation and continuous monitoring are essential to accurately capture and assess metrics like energy consumption, GHG emissions, and resource use in real-time (Kaewunruen, Peng, and Phil-Ebosie 2020; Tao et al. 2022).

Scope, intrinsically connected to granularity, is another significant factor. DT implementations generally target specific processes, yet achieving sustainability goals requires a broader scope encompassing the full operational boundaries of a firm (Abeysekera 2022).

Extending the functional boundaries of DT systems – conceptualised as nested systems within the manufacturing SoS – could significantly enhance holistic sustainability performance evaluation, supporting broader improvements from optimising process planning to reducing resource consumption and addressing occupational hazards.

Another challenge lies in aligning DT objectives and scale with SR requirements. Modifying or reusing existing DTs may be complex and resource intensive. Literature supports the notion that model development should be purpose-driven; therefore, evaluating the potential for purpose-built DTs tailored to SR is warranted. Such an evaluation might consider an integrated ‘two-in-one’ DT-SR system or an SR layer within a DT architecture. This approach would allow for adaptation while ensuring alignment with sustainability requirements, though its cost-effectiveness and scalability require investigation.

Finally, given the focus on sustainability, the potential environmental and social impacts of DTs itself warrant consideration. Manufacturing sustainability encompasses all energy consumption, thus the negative impacts of DTs cannot be neglected. The energy requirements and resource use for devices and software are non-trivial; however, the sustainability gains achievable through improved performance may offset these costs (Gundalini 2022; Tzachor et al. 2022). From a social perspective, DTs could impact employment dynamics, as increased automation will change traditional job roles, creating demand for new digital skills while reducing manual labour. Furthermore, concerns around data privacy and cybersecurity are increasingly relevant, as greater data integration and real-time monitoring may expose staff to increased risk and surveillance, impacting workplace privacy (Wang et al. 2023). As DT systems continue to evolve, the assessment of both their positive and negative impacts is essential to realising their potential in supporting sustainability goals ethically.

7. Conclusions and future work

7.1. Synthesis of findings and conceptual contribution

This research addressed a critical gap by investigating how manufacturing DTs and SR systems can be integrated. The literature review established that these domains operate as silos; DTs purpose-built for operational efficiency with incidental sustainability benefits and SR systems mandated by regulation yet dependent on manual data collection and estimation. Interview findings confirmed this reflects organisational and architectural barriers rather than technological constraints.

To address this, the study developed a structured, theoretically grounded framework for DT-SR integration through a SoS lens, where DT and SR systems integrated to enable emergent capabilities, i.e. real-time sustainability visibility and bidirectional optimisation. Such bidirectional capability challenges the prevailing characterisation of sustainability as a constraint, repositioning it as an optimisation opportunity by ensuring SR targets guide DT validated operational change.

The framework provides a systematic methodology for translating granular, process-level DT data into standardised, enterprise-level SR metrics. The four-step process framework of Mapping (identifying DT data sources and SR requirements), Matching (aligning process-level data to organisational metrics), Measuring (calculating sustainability indices), and Modelling (scenario analysis and decision support) provides actionable guidance. The proposed framework establishes a data governance roadmap that balances the operational need for data streams with the corporate requirement for auditable SR compliance. Specifically, the framework defines the links by which DT data informs SR. This offers practitioners a means of addressing the challenges identified in the expert interviews, demonstrating the practical utility of the framework for aligning operational efficiency with mandatory reporting.

The framework application represents proof-of-concept of the interfaces in simplified manufacturing contexts with idealised data availability and neutral organisational assumptions. The systematic specification of the framework integration provides actionable implementation guidance beyond conceptual contribution alone. It is important to note that the framework’s primary empirical domain is environmental sustainability metrics, including energy consumption, GHG emissions, water, and waste. Social and governance metrics are treated as partially within scope where they are digitally traceable within manufacturing system boundaries; however, their systematic integration requires further methodological development and lies beyond the current framework’s principal contribution.

7.2. Contributions to knowledge and practice

This work advances understanding of how improvements in sustainable manufacturing are explicitly linked to corporate sustainability performance, highlighting the methodological importance of designing the DT-SR integration interface within a SoS framework. It extends the scope of manufacturing modelling beyond direct production impact reduction to enterprise-level sustainability performance reporting.

The research demonstrates that DT-SR integration creates bidirectional value: efficiency gains become sustainability enhancements; sustainability targets become operationally implementable. This reconceptualization positions sustainability as an optimisation opportunity rather than a compliance constraint, with implications for how the manufacturing research community conceptualises the relationship between reporting objectives and competitive performance.

The proposed DT-SR framework shifts DTs from operational tools to tactical and potentially strategic management instruments. The identified value propositions directly address practitioners' current frustrations with system disconnection. Operations managers acknowledged that current DT platforms capture relevant sustainability data – energy consumption at machine level, material flows through processes, equipment utilisation patterns – yet lack mechanisms for translating this granular data into SR language. This gap represents both operational inefficiency (duplicating data collection) and missed opportunity (no real-time feedback enabling improvement). Our proposed DT-SR framework suggests a data governance structure to balance operational needs for continuous data with accountability needs through policies defining which DT data feeds SR. The managerial contribution offers organisations considering DT-SR integration a realistic roadmap addressing known barriers while capturing identified value propositions.

7.3. Future research

In response to the research question, 'How could manufacturing digital twins facilitate and enhance corporate sustainability reporting?', this study confirms the synergies and identifies imperative directions for future research. Figure 9 outlines key research areas and their intended contributions.

Firstly, empirical validation may begin with pilot studies that demonstrate proof of concept and technical feasibility, followed by multi-process, facility-scale, and cross-site implementations that explore scalability and contextual variation. Broader applications across sectors could reveal integration challenges and inform refinement of the framework. Enhancing DT capabilities for cause–effect reasoning and scenario analysis would contribute to more transparent and adaptive sustainability monitoring. Together, these studies can provide a stronger empirical basis for evaluating the scalability and generalizability of DT-SR integration. Comparability across pilots would benefit from a consistent set of evaluation benchmarks, including the share of mandatory SR disclosures traceable to DT sources without manual

supplement, deviation between DT-calculated and conventionally derived sustainability figures, SR preparation time savings relative to a pre-integration baseline, and evidence that DT feedback loops visibly inform subsequent operational adjustments. Adopting these benchmarks from the outset would allow findings from individual sites to be meaningfully accumulated into a generalisable evidence base. A tractable Phase 1 pilot would instrument a single manufacturing site, trace one ESRS E1 energy stream through all four framework steps, and evaluate outcomes against these benchmarks using a pre–post comparison of SR preparation time and manual data supplementation rates. The evaluation protocol should follow an embedded case study design (Yin 2014), with units of analysis at process, facility, and corporate levels, enabling systematic testing of whether DT-derived SR metrics align with conventionally derived figures across each level.

Secondly, theoretical development offers an opportunity to deepen insight into bidirectional DT-SR system behaviour. Building on a SoS foundation, the inclusion of CAS theory could clarify how operational fluctuations influence sustainability outcomes at multiple organisational levels. Future inquiry may model feedback loops and adaptive responses to understand how variability propagates through systems, how process-level efficiencies translate to higher-level sustainability metrics, and how feedback mechanisms enable ongoing adaptation. A combined SoS-CAS perspective can help refine theoretical propositions and boundary conditions, providing a stronger conceptual base for sustainable manufacturing systems.

Thirdly, scope and scale progression involves extending investigation across manufacturing hierarchies and organisational boundaries. Research progressing from single-process implementations to multi-site, inter-firm, and ecosystem levels can test whether facility-level improvements – such as reductions in energy use or waste – translate into measurable corporate or sectoral performance outcomes. Longitudinal analysis may clarify how sustainability gains evolve over time and across contexts. Moreover, an opportunity exists to broaden the scope of this study from manufacturing systems to supply chains and broader ecosystems. Applying the SoS framework to supply chains and industrial ecosystems positions DTs as distributed subsystems capable of coordinated monitoring, while also highlighting continuing challenges in data interoperability and governance.

Fourthly, although this study provides a conceptual framework for DT-SR integration from a data operations perspective, future work can focus on creating reusable interface design patterns that enable consistent

data exchange across systems and their processes. Further, there is the need to develop algorithms for temporal adaptation, boundary translation, and data synchronisation to ensure alignment between operational data and sustainability indicators. This includes the design of interoperable interfaces, development of temporal adaptation and synchronisation algorithms, and refinement of boundary translation methods to align DT data with established SR standards. Strengthening data governance – through validation, auditing, and decision-support protocols – would enable real-time optimisation and enhance transparency. To illustrate the specificity required: a temporal adaptation algorithm would need to aggregate per-cycle machine sensor readings (typically at second-level frequency) into the monthly and annual windows required by ESRS, applying documented gap-handling rules and preserving a full provenance log for audit; developing and validating such algorithms across different manufacturing contexts and SR standards is a concrete and necessary next step. These methodological refinements are foundational to establishing the necessary system-wide data governance frameworks across interconnected processes and sites.

Acknowledgements

The research work underlying this paper was conducted as part of the project 'Multiscale Digital Twin-Driven Smart Manufacturing System for High Value-Added Products project', which is funded by the UK's Engineering and Physical Sciences Research Council (EPSRC) with the project funding reference number EP/T024844/1. Additionally, we thank the contributing anonymous interviewees for their time and enthusiasm. The authors Yujia Luo (YL), Juan Ramon Candia (JRC) and Peter Ball (PB) made the following contributions based on the CRediT framework. Conceptualisation, PB (lead), YL and JRC (supporting); Methodology, JRC (lead), YL and PB (supporting); Investigation, YL and JRC (joint); Formal Analysis, YL and JRC (joint leads) and PB (supporting); Data Curation, YL and JRC (jointly); Writing – Original Draft, YL (lead), JRC and PB (supporting); Writing – Review & Editing, YL (lead), JRC and PB (supporting); Visualisation, YL and JRC (joint); Funding Acquisition, PB.

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CRediT: **Yujia Luo:** Conceptualization, Investigation, Visualization, Writing – original draft, Writing – review & editing; **Juan Ramón Candia:** Conceptualization, Investigation, Methodology, Visualization, Writing – original draft, Writing – review & editing; **Peter Ball:** Conceptualization, Funding acquisition, Investigation, Resources, Supervision, Validation, Writing – review & editing

Disclosure statement

No potential conflict of interest was reported by the author(s).

Funding

This work was supported by Engineering and Physical Sciences Research Council [grant number EP/ T024844 /1].

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Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request. This excludes interview transcripts as they contextually could

enable identification of interviewees which would breach the anonymity guarantees given to them. Anonymized excerpts are available in Appendix 4; further anonymized excerpts may be provided under a data-sharing agreement upon reasonable request.

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Appendices

Appendix 1. Topics and subtopics considered by ESRS

Standard	Topic	Sub-Topic
ESRS E1	Climate Change	- Climate change adaptation - Climate change mitigation
ESRS E2	Pollution	- Energy - Pollution of air - Pollution of water - Pollution of soil - Pollution of living organisms and food resources - Substances of concern - Substances of very high concern
ESRS E3	Water and marine resources	- Microplastics - Water consumption - Water withdrawals - Water discharges - Water discharges in the oceans
ESRS E4	Biodiversity and ecosystems	- Extraction and use of marine resources - Direct impact drivers of biodiversity loss (e.g. climate change, land-use change, fresh water-use change, direct exploitation, pollution, others) - Impacts on the state of species (e.g. population size, global extinction risk). - Impacts on the extent and condition of ecosystems (e.g. land degradation, desertification).
ESRS E5	Circular economy	- Impacts and dependencies on ecosystem services - Resources inflows, including resource use - Resource outflows related to products and services
ESRS S1	Own workforce	- Waste - Working conditions (e.g. secure employment, working time, adequate wages, social dialogue) - Equal treatment and opportunities for all (e.g. gender equality, training).
ESRS S2	Workers in the value chain	- Other work-related rights (e.g. child labour, forced labour) - Working conditions (e.g. secure employment, working time, adequate wages). - Equal treatment and opportunities for all (e.g. gender equality, training).
ESRS S3	Affected communities	- Other work-related rights (e.g. child labour, forced labour) - Communities' economic, social and cultural rights - Communities' civil and political rights
ESRS S4	Consumers and end- users	- Rights of indigenous peoples - Information-related impacts for consumers and/or end-users - Personal safety of consumers and/or end-users
ESRS G1	Business conduct	- Social inclusion of consumers and/or end-users - Corporate culture - Protection of whistle-blowers - Animal welfare - Political engagement and lobbying activities - Management of relationships with suppliers including payment practices - Corruption and bribery

Source: European Parliament (2024).

Appendix 2. Examples of metrics contained in ESRS standards – topic environment, ESRS E1 (EFRAG, Nov. 2022)

ESRS E1 Climate Change

Energy consumption and mix Comparative Year N

- (1) Fuel consumption from coal and coal products (MWh)
- (2) Fuel consumption from crude oil and petroleum products (MWh)
- (3) Fuel consumption from natural gas (MWh)
- (4) Fuel consumption from other non-renewable sources (MWh)
- (5) Consumption from nuclear products (MWh)
- (6) Consumption of purchased or acquired electricity, heat, steam, and cooling from non-renewable sources (MWh)
- (7) Total non-renewable energy consumption (MWh) (calculated as the sum of lines 1 to 6) Share of non-renewable sources in total energy consumption (%)
- (8) Fuel consumption from renewable sources (including biomass, biogas, non-fossil fuel waste, renewable hydrogen, etc.) (MWh)
- (9) Consumption of purchased or acquired electricity, heat, steam, and cooling from renewable sources (MWh)
- (10) The consumption of self-generated non-fuel renewable energy (MWh)
- (11) Total renewable energy consumption (MWh) (calculated as the sum of lines 8 to 10) Share of renewable sources in total energy consumption (%)
- Total energy consumption (MWh) (calculated as the sum of lines 7 and 11)
- Energy intensity per net revenue Comparative
- Total energy consumption from activities in high climate impact sectors per net revenue from activities in high climate impact sectors (MWh/Monetary unit)

2. How can sustainability values and metrics be integrated in digital twins to achieve the sustainability goals of companies?
3. What are the limitations of digital twins and existing measurements in the context of addressing sustainability requirements?
4. How aggregated/desegregated is the info companies use for their sustainability reports?
5. How standardised are the various methodologies for calculations? (e.g. water usage, carbon emissions, circularity, biodiversity, etc.)
6. What sustainability data do you incorporate in DT? For example, energy consumption in machines (individual machines, the whole system, etc).
7. How is the process for getting that data, how do you validate it, etc.
8. What is the system boundary? (The system boundary could evolve to expand beyond site-specific facilities to encompass value chain thinking)
9. Do you think the social and governance aspects of CSRD can be integrated in DTs (or some of them)? Given the European Sustainability Reporting Standards (ESRS), S1 through S4, cover workforce conditions, value chain workers, affected communities, and consumers, measuring parameters like working conditions, equal treatment, and social inclusion. ESRS G1 addresses corporate culture, whistle-blower protection, animal welfare, political engagement, supplier relationships, and anti-corruption measures.

Appendix 3. Interviews questions

1. How could DTs facilitate and enhance SPR in the manufacturing sector?

Appendix 4. Interview quotes

Table A1. Quotes from interviewees regarding data availability and data quality.

Interviewees Quotes	Company
We need to identify which aspects of sustainability are going to be related to DT. Environmental sustainability is easier than social sustainability, because the metrics are related to quantities of things.	Company A
Issue of granularity. Can be really detailed? e.g for product centric evaluation. We need to evaluate the value of getting this information, is it worth it?	Company A
Most organisations will have only one metre for water and for energy for the whole site or building. So to generate data at a product level, implies generating data that doesn't currently exist.	Company A
Is DT going to help reporting slavery? as these aspects are not necessarily related to the manufacturing process. Maybe when it comes to the internal workforce there could be an overlap.	Company A
Customers are struggling to get the needed data to feed into the system, they can often get it as an estimate for the whole factory, when the factory is running normally, but they struggle at a more granular level.	Company B
DT work best whenever they've got high quality data. One of the things that we are experiencing across our clients is the challenges around data sharing between different organisations (due to different formats, lack of data, unwillingness to share, lack of capacity).	Company C
Also a knowledge gap within some companies of what is good enough. So there's that sort of trade-off between availability and quality ... Also a high dependency on others (suppliers), with low quality data, low frequency. But it's a very laborious process and the data is not great (use of proxy data rather than actual really effective data from metering)	Company C
I think the level of maturity that we've seen at the moment to enable the embedding DT and CSRD system and the marriage of the requirements with a digital twin is probably not there.	Company C
I think some of the constraints we've seen, is the lack of cross sector collaboration on data collection and the lack of standardisation that hopefully some of these pieces of regulation are going to start to solve. In terms of the new legislation (CSRD), there's enthusiasm and a willingness by companies to push forward, but there's a bit of frustration and also nervousness around.	Company C
So this is the million dollar question, how do we standardise data formats, how do we kind of enable open data sharing? And then how are we going to actually get that data? What's the technology that will enable that process? So it's really complex.	Company C
I think people would massively see the benefit of DT if you can reduce the reporting burden, the manual aspect of it. But what they would need is to trust the quality of the data and maybe to put in some form of assurance through the process.	Company C
So for the case that I'm talking about, that data essentially didn't exist at the level of detail needed. So what we actually did was we used a simulation model.	Company D
If you're using simulated data, there needs to be some level of explainability and how that data is being produced. So what are the set of assumptions? If you are able to get data, what's the relationship between the actual versus the simulated, normally called the sim to real gap.	Company D
And again, that comes down to the data and availability and what it's able to actually report on, realistically. So, and in terms of the sustainability side of it, I think that's even harder because as we said at the beginning, you know, people reporting on sustainability are normally reporting on a per quarter basis or a per annum basis or whatever it might be.	Company D

Table A2. Quotes from interviewees regarding use of data for decision making.

Interviewees Quotes	Company
More often business questions are around risks, avoid risks. Risk is the entry point. Some of these decisions maybe be related to sustainability metrics, but it still is a financial reasoning behind, about investments.	Company B
Simulation could play a good role in making a business case for optimisation. If you have these sensors, you get this level of data, which can help make different decisions. DT is operational, and if you can use it to optimise e.g. running the furnace at night, it could be a more sustainable option as well (optimisation). But simulation is a great tool for investments.	Company B
Companies may need a use case to better understand and clarify the potential for DT, and also its relationship with sustainability performance and reporting. If they could see there is a feedback loop between presenting these metrics, taking action and getting the benefits, that is a use case to implement DT, but they need to see that feedback loop will have an impact.	Company B
There's no point building a DT that is just about sustainability metrics. You have to build it so that it has considerations of those other bits so that if people are making a decision, they can see the benefit to the other bits of the business, by making certain decisions (what would it do to cost efficiency, level of resource use, like these sorts of aspects).	Company C
What decisions do you need to make? What level of confidence do you need in these decisions? let's not make all of this about just reporting. Let's make sure it is still useful and driving decision making. If we're going to have to do this for reporting, can we figure out how we can use it to enhance our customer experience or maybe augment our value proposition	Company C
We have observed that people don't necessarily have the capability to interpret sustainability data across the multitude of factors that come with environmental sustainability. So how do they make trade-off decisions between carbon and waste, for example. How do we help people interpret those trade-offs (within DT development). A lot of it will hopefully be guided by materiality assessments through the CSRD process, it should hopefully give a level of insight for companies in terms of how they prioritise that type of decision making around trade-offs.	Company C
I see digital twins being incorporated into that broader AI Convergence of lots of different techniques and digital twins is one aspect of that, because it's essentially the combination of different what I would call composite techniques, so simulation mixed with optimisation mixed with machine learning and that's what produces potentially your digital twin and the data architecture that goes behind it that's feeding in data at an interval that makes sense.	Company D
I think it needs to be made for non expert users, and that's something that I think is going to take a lot more time than, than actually building the models because those models exist and have existed for a little while now	Company D
In terms of the question about sustainability, many of the models we have been working on focussed on not just from the capacity point of view, how do we balance the level of production that is required, but also with the increasing sustainability requirements that have been set, from compulsory point of view. That included measuring the amount of waste produced within the system and minimising that, as well as making the processes as efficient as possible. Also considered the energy aspect (energy mix between renewables and energy pull from the grid). But it does require the actual data pipeline, the detail of that data (granularity) to work consistently with the production system	Company D