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Digital Twin-Enabled Cybersecurity Architecture for Predicting, Simulating, and Mitigating Advanced Persistent Threats Across Smart Manufacturing Systems

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Abstract: The accelerating digitalisation of industrial operations has transformed manufacturing into a highly interconnected ecosystem driven by Industrial Internet of Things (IIoT), cyber-physical systems, cloud computing, edge intelligence, and artificial intelligence. While these technological advancements have improved automation, operational efficiency, and real-time decision-making, they have also introduced increasingly complex cybersecurity challenges arising from expanded attack surfaces, interconnected assets, and continuously evolving threat landscapes. Among these threats, Advanced Persistent Threats (APTs) pose a particularly significant risk due to their stealth, persistence, and ability to infiltrate critical manufacturing infrastructure through multi-stage attack campaigns that often evade conventional security mechanisms. Existing cybersecurity solutions predominantly adopt reactive detection and response strategies, limiting their effectiveness in anticipating sophisticated attacks before operational disruption occurs. This study proposes a Digital Twin-enabled cybersecurity architecture for predicting, simulating, and mitigating Advanced Persistent Threats across smart manufacturing systems. The proposed framework integrates continuously synchronised digital twins with real-time operational data, AI-driven anomaly detection, attack graph modelling, behavioural analytics, and cyber-attack simulation to identify vulnerabilities, forecast attack progression, evaluate mitigation strategies, and support adaptive security decision-making without interrupting physical operations. Furthermore, the study presents a comprehensive architectural and performance evaluation framework that demonstrates how Digital Twin technology can strengthen cyber resilience, enhance threat preparedness, optimise incident response, and safeguard the reliability, continuity, and security of next-generation smart manufacturing environments.
Keywords: Digital Twin; Advanced Persistent Threats; Smart Manufacturing; Industrial Cybersecurity; Attack Simulation; Cyber Resilience

1. INTRODUCTION

1.1 Digital Transformation of Smart Manufacturing and Emerging Cybersecurity Challenges

The manufacturing sector has undergone a profound digital transformation over the past decade, transitioning from conventional automation towards highly interconnected and intelligent production environments characterised by the principles of Industry 4.0 [1]. Unlike traditional manufacturing systems that relied on isolated production equipment and centralised control architectures, modern smart factories integrate Industrial Internet of Things (IIoT) devices, Cyber-Physical Systems (CPS), artificial intelligence (AI), cloud computing, edge computing, robotics, and industrial automation into unified digital ecosystems capable of supporting autonomous decision-making and real-time operational optimisation [2]. These technologies enable continuous monitoring of manufacturing assets, predictive maintenance, adaptive production scheduling, quality assurance, and resource optimisation while improving operational efficiency, flexibility, and product customisation [3].

The convergence of digital technologies has expanded manufacturing beyond individual production facilities into interconnected ecosystems comprising suppliers, logistics providers, cloud platforms, industrial control systems, enterprise resource planning applications, and remotely managed production assets [4]. Continuous exchange of operational data among these heterogeneous components enhances collaboration and productivity but simultaneously increases system complexity and dependence on digital communication infrastructures [5]. Consequently, manufacturing organisations now operate within cyber-physical environments where disruptions affecting digital components can rapidly propagate to physical production processes, resulting in equipment failures, operational downtime, compromised product quality, and supply-chain interruptions [2].

The growing connectivity of smart manufacturing environments has substantially expanded the cyber attack surface available to malicious actors [6]. IIoT devices, programmable logic controllers, industrial communication protocols, cloud services, edge devices, and remote maintenance interfaces introduce multiple entry points that can be exploited through sophisticated cyber intrusions [7]. The resulting cyber incidents often extend beyond financial losses to include production disruption, intellectual property theft, safety risks, reputational damage, and reduced industrial competitiveness, highlighting cybersecurity as a strategic requirement for resilient smart manufacturing systems [8].

1.2 Advanced Persistent Threats as a Critical Risk to Smart Manufacturing Systems

Among the numerous cybersecurity threats confronting Industry 4.0 environments, Advanced Persistent Threats (APTs) represent one of the most sophisticated and damaging categories of cyber attacks targeting industrial organisations [9]. Unlike opportunistic cyber intrusions, APTs are characterised by long-term persistence, stealth, targeted objectives, and highly coordinated attack strategies designed to evade conventional security mechanisms while maintaining continuous access to critical systems [2]. Attackers typically employ multiple techniques, including social engineering, credential theft, zero-day vulnerabilities, malware deployment, lateral movement, privilege escalation, and covert command-and-control communication to compromise industrial assets over extended periods without detection [6].

The lifecycle of an APT generally progresses through reconnaissance, initial compromise, persistence establishment, privilege escalation, lateral movement, intelligence collection, operational manipulation, and objective execution [1]. Within smart manufacturing environments, these attacks frequently target proprietary production processes, industrial control systems, product designs, operational technologies, and confidential manufacturing knowledge to facilitate industrial espionage, competitive advantage, or geopolitical objectives [5]. Modern manufacturing supply chains further increase organisational exposure because compromise of trusted software vendors, equipment manufacturers, or service providers can provide attackers with indirect access to multiple production environments simultaneously [9]. In addition, attacks against critical manufacturing infrastructure may disrupt production continuity, damage industrial equipment, compromise worker safety, and interrupt national supply chains supporting essential economic sectors [3].

Despite significant advances in industrial cybersecurity, conventional intrusion detection systems (IDS), intrusion prevention systems (IPS), security information and event management (SIEM) platforms, and rule-based detection mechanisms remain largely reactive and signature-dependent [7]. These approaches often struggle to detect previously unseen attack behaviours, correlate complex multi-stage intrusion activities, or anticipate future attack progression, limiting their effectiveness against adaptive and persistent cyber adversaries operating within dynamic smart manufacturing ecosystems [4].

1.3 Research Gap, Aim, Objectives and Contributions

Although artificial intelligence, behavioural analytics, and industrial monitoring technologies have strengthened manufacturing cybersecurity, existing approaches remain predominantly reactive, fragmented, and insufficiently integrated with continuously evolving cyber-physical manufacturing processes [2]. Most current security frameworks focus on detecting individual attack events after compromise has occurred rather than providing predictive capabilities capable of simulating attacker behaviour, assessing evolving system vulnerabilities, and recommending proactive mitigation strategies across interconnected manufacturing environments [7]. Digital Twin technology offers a promising alternative by creating dynamic virtual representations of physical manufacturing systems that continuously synchronise operational data, enabling real-time cyber risk modelling, attack simulation, anomaly detection, and predictive decision support [5].

This study therefore aims to develop a Digital Twin-enabled cybersecurity architecture for predicting, simulating, and mitigating Advanced Persistent Threats across smart manufacturing systems. The specific objectives are to design an integrated Digital Twin cybersecurity framework, develop mathematical models for dynamic threat prediction and attack propagation, investigate intelligent mitigation strategies for multi-stage cyber attacks, and establish quantitative performance metrics for evaluating cyber resilience and operational security. The scope of the study encompasses Industry 4.0 manufacturing environments incorporating cyber-physical production systems, IIoT devices, cloud-edge infrastructures, and industrial communication networks. The principal contributions include an integrated Digital Twin cybersecurity architecture, advanced mathematical formulations for predictive threat modelling, intelligent optimisation techniques for adaptive defence, and a comprehensive evaluation framework supporting resilient industrial cybersecurity.

2. LITERATURE REVIEW AND THEORETICAL FOUNDATIONS

2.1 Evolution of Industrial Cybersecurity in Smart Manufacturing

Industrial cybersecurity has evolved substantially in response to the increasing digitalisation of manufacturing systems and the convergence of operational technology (OT) with information technology (IT) environments [9]. Early industrial control systems (ICS) were designed primarily for reliability, availability, and operational continuity rather than cybersecurity because they operated as isolated networks with limited external connectivity [12]. Security mechanisms therefore focused on physical access control, proprietary communication protocols, and perimeter isolation, assuming that industrial environments would remain largely disconnected from public networks [7]. However, the rapid adoption of Industry 4.0 technologies, cloud services, remote maintenance, Industrial Internet of Things (IIoT) devices, and interconnected manufacturing platforms has fundamentally altered this security paradigm by exposing industrial systems to increasingly sophisticated cyber threats [14].

Supervisory Control and Data Acquisition (SCADA) systems, which provide centralised monitoring and control of distributed industrial processes, initially relied on firewalls, network segmentation, and access control mechanisms to reduce unauthorised system access [10]. As cyber threats evolved, the convergence of OT and IT infrastructures

introduced new attack vectors through enterprise networks, cloud platforms, mobile devices, and third-party service providers, necessitating integrated cybersecurity strategies capable of protecting both operational processes and digital information assets [15]. This convergence has encouraged the adoption of Zero Trust security architectures that continuously verify user identities, device integrity, and application behaviour instead of assuming implicit trust within industrial networks [8].

Recent advances in artificial intelligence have further transformed industrial cybersecurity by enabling anomaly detection, behavioural analytics, automated threat hunting, and predictive risk assessment using large-scale operational data [11]. These intelligent capabilities support industrial cyber resilience by facilitating continuous monitoring, adaptive defence, rapid incident response, and proactive recovery across increasingly interconnected smart manufacturing environments [13].

2.2 Digital Twin Technology for Industrial Systems

Digital Twin technology has emerged as one of the defining innovations supporting intelligent manufacturing by enabling continuous synchronisation between physical industrial assets and their virtual representations throughout the asset lifecycle [13]. Although early digital engineering models primarily supported product design and simulation, modern Digital Twins integrate real-time operational data, computational intelligence, and predictive analytics to create dynamic virtual environments capable of reflecting continuously changing manufacturing conditions [8]. Advances in Industrial Internet of Things (IIoT) connectivity, high-speed communication networks, cloud computing, and edge intelligence have significantly enhanced the fidelity and responsiveness of Digital Twin systems, allowing physical processes to be monitored, analysed, and optimised in near real time [15].

Physical–virtual synchronisation forms the foundation of Digital Twin technology by continuously integrating telemetry acquired from industrial sensors, programmable logic controllers, machine tools, robotics, environmental monitoring devices, and enterprise information systems into an evolving digital representation of manufacturing operations [10]. This bidirectional exchange enables operational changes within physical systems to be reflected immediately within the virtual environment while analytical insights generated by the Digital Twin can inform maintenance planning, production scheduling, and process optimisation [7]. Continuous telemetry further supports predictive monitoring by identifying equipment degradation, abnormal operating conditions, and emerging system anomalies before they develop into production failures or safety incidents [12].

Beyond monitoring, Digital Twins provide powerful industrial simulation capabilities that enable engineers to evaluate alternative operational strategies, assess equipment performance, simulate fault propagation, and analyse cyber-physical interactions without disrupting live manufacturing processes [9]. These simulation capabilities strengthen decision support by allowing organisations to evaluate potential interventions, optimise resource utilisation, reduce operational uncertainty, and improve manufacturing resilience through evidence-based planning and intelligent operational control [14].

2.3 Advanced Persistent Threat Modelling and Cyber Kill Chain Analysis

Advanced Persistent Threats (APTs) are distinguished from conventional cyber attacks by their strategic planning, prolonged persistence, adaptive behaviour, and clearly defined objectives, making them particularly difficult to detect within interconnected smart manufacturing environments [11]. Unlike signature-based attacks that exploit isolated vulnerabilities, APTs evolve through coordinated stages that enable attackers to establish persistence, evade detection, move laterally across industrial networks, and ultimately compromise critical manufacturing assets or intellectual property [8]. Understanding this progression requires structured threat-modelling frameworks capable of describing attacker behaviour across the entire intrusion lifecycle rather than focusing on individual attack events [14].

The MITRE ATT&CK framework provides a comprehensive knowledge base of adversarial tactics, techniques, and procedures (TTPs), enabling defenders to associate observed system behaviours with known attack methodologies across enterprise and industrial environments [9]. Complementing this approach, the Cyber Kill Chain decomposes an attack into sequential phases, including reconnaissance, weaponisation, delivery, exploitation, installation, command-and-control, and actions on objectives, thereby enabling organisations to identify appropriate defensive measures at each stage of an intrusion [15]. The Diamond Model of Intrusion Analysis further characterises cyber attacks by analysing the relationships among adversaries, infrastructure, capabilities, and victims, providing contextual intelligence that supports attribution, behavioural analysis, and threat correlation [7].

Graph-based attack modelling extends these approaches by representing cyber attacks as interconnected attack graphs that capture possible intrusion paths across industrial assets and communication networks [13]. Combined with behaviour-based threat intelligence, these models enable continuous identification of abnormal activities, adaptive attack progression, and emerging threat patterns using operational telemetry instead of relying solely on predefined signatures [10]. Consequently, modern APT modelling provides the analytical foundation required for predictive cyber defence, proactive threat hunting, and intelligent mitigation within Digital Twin-enabled manufacturing systems [12].

2.4 Existing Digital Twin Security Frameworks: Strengths, Limitations and Research Opportunities

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Recent advances in Digital Twin technology have stimulated the development of numerous cybersecurity frameworks designed to improve monitoring, simulation, and operational resilience across smart manufacturing environments [13]. Existing architectures commonly integrate Industrial Internet of Things (IIoT) devices, Cyber-Physical Systems (CPS), cloud platforms, and industrial communication networks to provide continuous visibility into manufacturing operations and facilitate predictive maintenance, operational optimisation, and anomaly detection [10]. Several frameworks further incorporate artificial intelligence to automate fault diagnosis, behavioural monitoring, and cyber anomaly detection, thereby improving operational awareness compared with conventional industrial security approaches [8].

Despite these advances, most existing Digital Twin security frameworks remain primarily descriptive, concentrating on system monitoring and post-event analysis rather than comprehensive predictive cybersecurity [15]. AI integration frequently focuses on isolated anomaly detection models without considering coordinated multi-stage attack progression, adversarial adaptation, or intelligent mitigation planning across interconnected industrial assets [9]. Similarly, although simulation capabilities enable engineers to evaluate operational scenarios and equipment performance, relatively few frameworks simulate dynamic cyber attack propagation or integrate attacker behaviour models derived from established threat intelligence frameworks such as MITRE ATT&CK or the Cyber Kill Chain [11]. Consequently, predictive intelligence remains fragmented, limiting the ability of existing Digital Twins to anticipate evolving cyber threats before operational disruption occurs [14].

These limitations reveal several important research opportunities. Future Digital Twin security architectures should integrate predictive threat modelling, behaviour-based cyber intelligence, adaptive mitigation strategies, hardware-aware artificial intelligence, and continuous cyber-physical synchronisation within a unified framework capable of supporting real-time cybersecurity decision-making [7]. Addressing these gaps provides the motivation for the Digital Twin-enabled predictive cybersecurity architecture proposed in this study, which combines intelligent simulation, adaptive defence, and quantitative performance evaluation to strengthen cyber resilience in smart manufacturing systems [12].

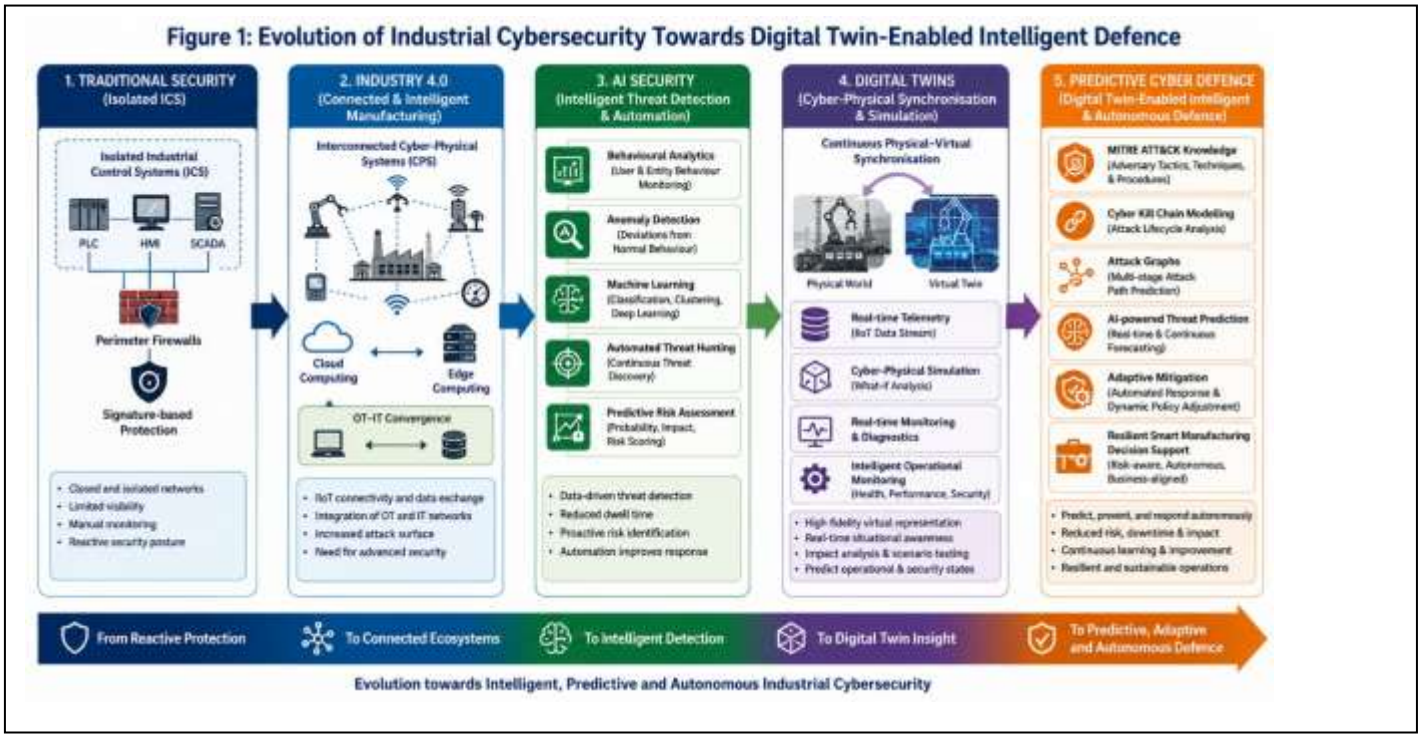

Table 1. Comparative Analysis of Existing Digital Twin-Based Cybersecurity Frameworks for Smart Manufacturing

Framework Characteristics	Digital Twin Monitoring	AI Integration	Cyber Attack Simulation	Predictive Intelligence	Adaptive Mitigation	Principal Limitation
Conventional	High	Limited	Low	Low	No	Primarily descriptiv

Framework Characteristics	Digital Twin Monitoring	AI Integration	Cyber Attack Simulation	Predictive Intelligence	Adaptive Mitigation	Principal Limitation
Digital Twin Architecture						e monitoring
AI-Enhanced Digital Twin	High	Moderate	Limited	Moderate	Partial	Focuses mainly on anomaly detection
Simulation-Based Digital Twin	Moderate	Limited	High	Low	No	Weak integration with real-time operational data
Industrial CPS Security Framework	Moderate	Moderate	Limited	Moderate	Partial	Limited cyber-physical synchronisation
Cloud-Based Digital Twin Security	High	Moderate	Moderate	Moderate	Partial	High communication latency and privacy concerns
Proposed Digital Twin Cybersecurity Architecture	High	Advanced	Advanced	High	Comprehensive	Integrated predictive defence and adaptive mitigation

3. PROPOSED DIGITAL TWIN-ENABLED CYBERSECURITY ARCHITECTURE

3.1 Overall System Architecture

The proposed Digital Twin-enabled cybersecurity architecture adopts a layered design that integrates cyber-physical manufacturing assets, intelligent analytics, and automated cyber defence into a unified operational framework capable of supporting predictive cybersecurity across Industry 4.0 environments [17]. Unlike conventional security architectures that monitor isolated events, the proposed system establishes continuous interaction between physical manufacturing processes, digital representations, artificial intelligence, and adaptive response mechanisms to improve cyber situational awareness and resilience [14]. Each architectural layer performs specialised functions while exchanging information with adjacent layers to support real-time threat prediction and coordinated defensive decision-making [20].

The Physical Manufacturing Layer comprises production equipment, programmable logic controllers, robotic systems, industrial control systems, sensors, actuators, conveyors, and manufacturing assets responsible for executing operational processes [13]. Above this layer, the Industrial Internet of Things (IIoT) Layer acquires operational telemetry from distributed sensors, machine controllers, smart devices, and industrial gateways, providing continuous observations describing equipment behaviour and production status [22]. The Communication Layer enables secure data transmission through industrial Ethernet, wireless industrial networks, time-sensitive networking, and cloud-edge communication infrastructures while supporting interoperability among heterogeneous manufacturing components [16].

The Digital Twin Layer maintains continuously synchronised virtual representations of physical assets by integrating operational telemetry, equipment models, production history, and cyber events into dynamic digital replicas capable of reflecting current manufacturing conditions [19]. The AI Analytics Layer performs anomaly detection, behavioural modelling, predictive analytics, graph learning, and probabilistic threat assessment using continuously updated Digital Twin information [15]. Intelligence generated within this layer is enriched by the Threat Intelligence Layer, which incorporates behavioural indicators, attack signatures, adversarial tactics, MITRE ATT&CK knowledge, and Cyber Kill Chain relationships to improve predictive cyber defence [21]. Finally, the Decision Support Layer prioritises defensive actions, while the Security Orchestration Layer coordinates automated mitigation, dynamic isolation, recovery planning, policy optimisation, and continuous learning to establish an adaptive cybersecurity ecosystem capable of protecting smart manufacturing operations against evolving Advanced Persistent Threats [18].

3.2 Real-Time Digital Twin Synchronisation and Cyber Situational Awareness

Effective cyber defence within smart manufacturing requires continuous awareness of evolving operational conditions across physical equipment, communication networks, and digital infrastructure rather than periodic security assessments [20]. The proposed framework therefore employs continuous Digital Twin synchronisation to maintain an accurate and dynamically updated representation of manufacturing operations using heterogeneous data acquired from industrial sensors, machine controllers, programmable logic controllers, network devices, enterprise systems, and cybersecurity monitoring platforms [14]. Multimodal sensor fusion combines telemetry collected from diverse sources to improve observation reliability, reduce uncertainty, and provide

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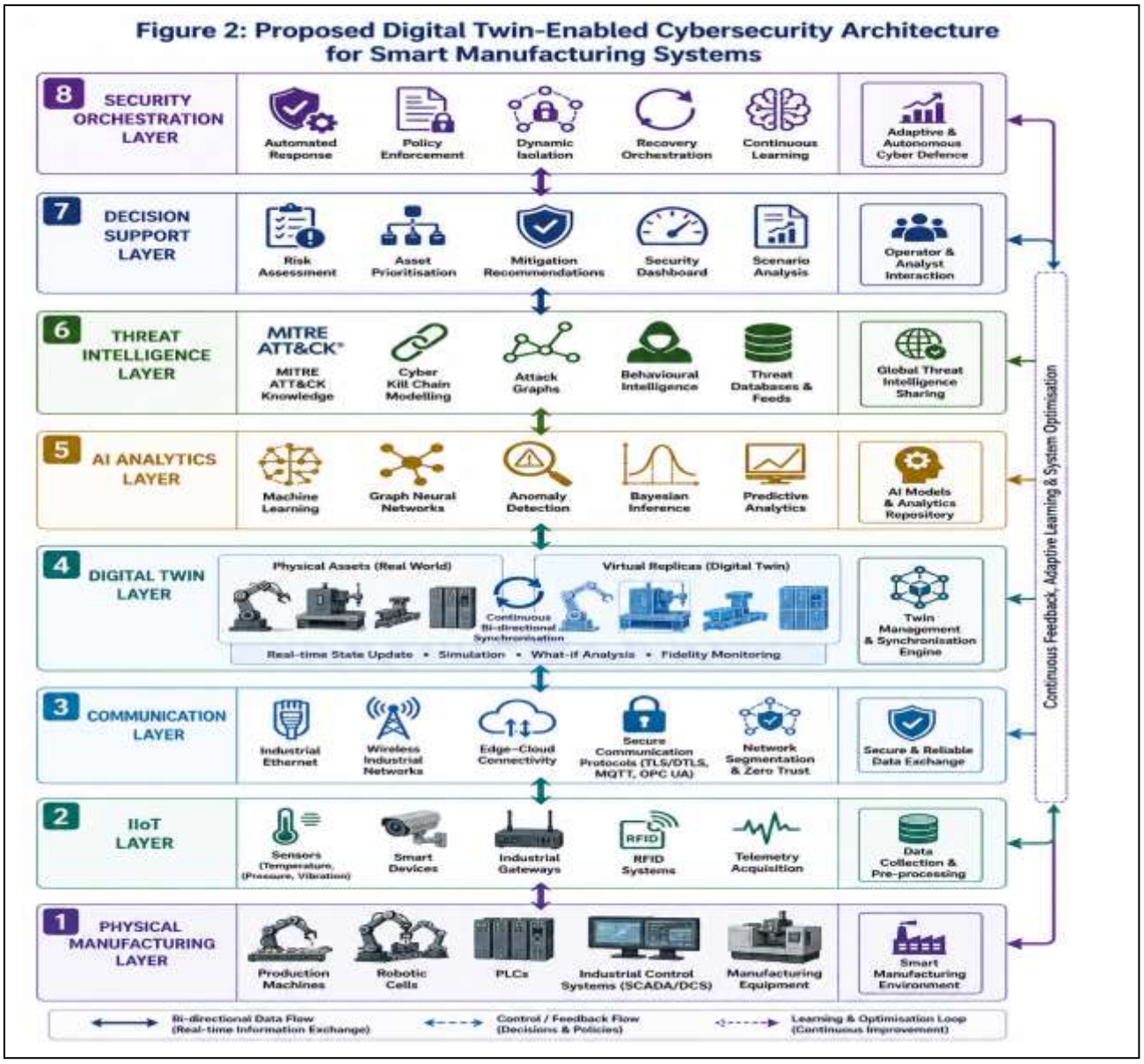
comprehensive visibility into manufacturing processes and cyber activities [17].

The Digital Twin continuously acquires operational data through distributed IIoT devices, communication gateways, industrial protocols, and network monitoring systems before integrating these observations into a unified cyber-physical representation [13]. State estimation algorithms evaluate equipment conditions, production behaviour, network performance, user activities, and cybersecurity events to maintain an accurate representation of manufacturing operations despite sensor noise, communication delays, or incomplete observations [21]. Continuous synchronisation ensures that changes occurring within physical manufacturing systems are immediately reflected within the Digital Twin, operating modes, maintenance history, user privileges, and network status when interpreting observed events, thereby reducing false alarms and improving threat detection accuracy [22].

The evolution of the Digital Twin is represented as

$$DT(t) = f(P(t), S(t), N(t), C(t))$$

where $P(t)$denotes the physical manufacturing state, $S(t)$represents sensor observations, $N(t)$describes network conditions, and $C(t)$captures the cybersecurity state of the manufacturing environment [16]. This formulation enables continuous behaviour monitoring and provides the dynamic foundation for predictive threat analysis, attack simulation,



enabling predictive analysis and rapid identification of abnormal behaviour before operational disruption occurs [18]. Context awareness further enhances cyber situational awareness by incorporating production schedules, equipment and adaptive cyber defence developed in the subsequent sections [19].

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3.3 AI-Driven Threat Prediction and Attack Path Simulation

The predictive capability of the proposed architecture is achieved by integrating multiple artificial intelligence techniques that collectively identify, forecast, and simulate Advanced Persistent Threats (APTs) before they compromise manufacturing operations [18]. Unlike conventional security systems that analyse isolated security events, the proposed framework continuously learns relationships among manufacturing assets, communication networks, user activities, and historical cyber incidents to anticipate future attack behaviour and recommend proactive defensive actions [15]. Machine learning algorithms establish behavioural baselines for production equipment, programmable logic controllers, industrial communication protocols, and user interactions, enabling early detection of deviations that may indicate malicious activity [20]. These continuously updated models improve detection accuracy by adapting to evolving operational conditions and reducing false-positive alarms generated by static rule-based approaches [13].

Graph Neural Networks (GNNs) further enhance predictive intelligence by modelling manufacturing systems as interconnected cyber-physical graphs in which machines, controllers, sensors, servers, and communication devices represent nodes linked through operational and network relationships [21]. Instead of analysing assets independently, GNNs propagate information across neighbouring nodes to identify hidden attack dependencies, estimate cascading compromise pathways, and evaluate how local vulnerabilities may propagate throughout an industrial environment [17]. Bayesian inference complements graph learning by continuously updating threat probabilities whenever new evidence becomes available from intrusion detection systems, network telemetry, Digital Twin observations, or behavioural analytics, thereby supporting uncertainty-aware cybersecurity decision-making [22].

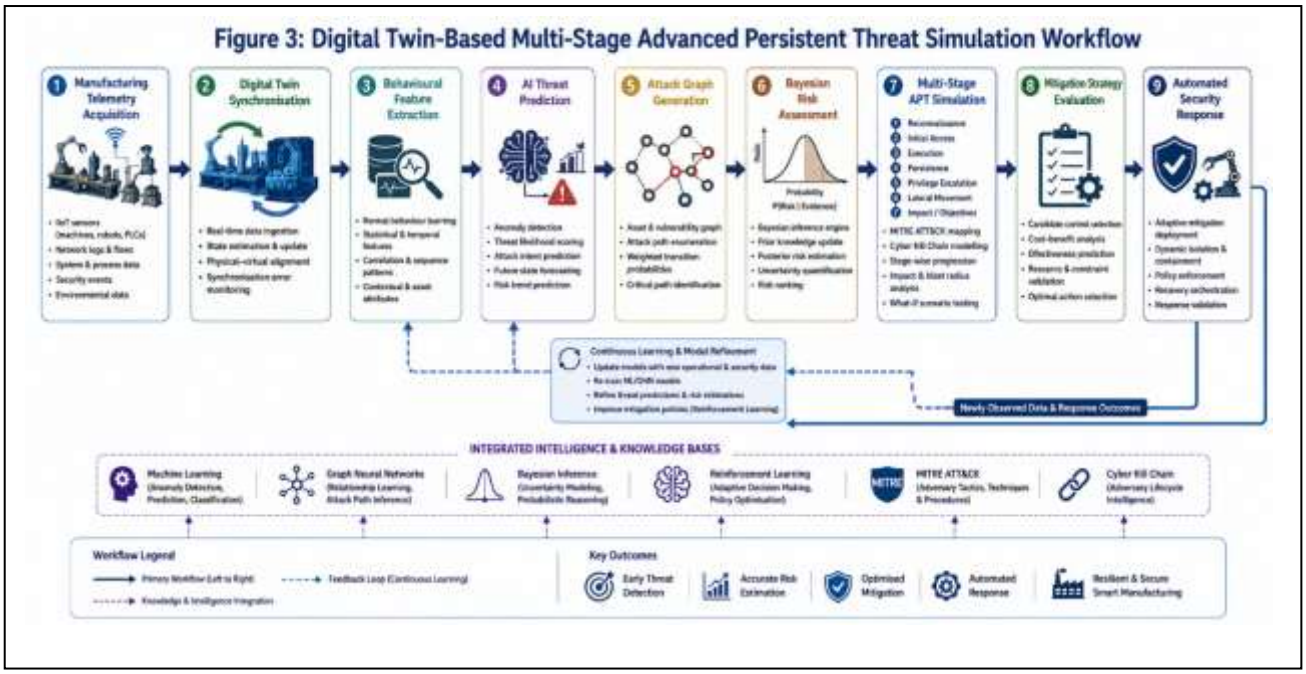
Attack propagation is modelled through attack graphs representing multiple intrusion pathways from initial compromise to mission objectives. Assuming successive attack stages are conditionally dependent, the probability of a complete attack sequence is approximated as

$$P(A) = \prod_{i=1}^{n} P_i,$$

where P_i denotes the probability of successfully completing attack stage i[14]. As additional operational evidence becomes available, attack likelihoods are revised using Bayes' theorem

$$P(H \mid E) = \frac{P(E \mid H)P(H)}{P(E)},$$

where H represents a threat hypothesis and E denotes newly observed cyber evidence [19]. Reinforcement learning further improves prediction by evaluating simulated attacker–defender interactions inside the Digital Twin, allowing defensive strategies to adapt continuously as attack behaviour evolves [16]. Consequently, the proposed framework supports multi-stage attack forecasting, proactive cyber defence, and intelligent mitigation before operational disruption occurs [18].



3.4 Adaptive Cyber Defence and Automated Response Framework

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Accurate threat prediction alone is insufficient for protecting smart manufacturing systems unless it is accompanied by intelligent and timely defensive actions capable of limiting attack progression and restoring secure operations [20]. The proposed architecture therefore incorporates an adaptive cyber defence framework that transforms predictive intelligence into automated mitigation strategies through continuous observation, risk evaluation, response orchestration, and learning [13]. Unlike conventional incident-response procedures that depend heavily on manual intervention, the proposed framework dynamically coordinates defensive actions according to attack severity, asset criticality, production requirements, and operational risk [22].

Following threat prediction, the framework automatically identifies affected manufacturing assets and determines appropriate containment measures, including dynamic network isolation, access-control modification, workload migration, process segmentation, and temporary suspension of compromised industrial services [17]. Asset prioritisation ensures that production systems supporting safety-critical operations, high-value manufacturing processes, and essential industrial services receive immediate protection before less critical resources [15]. Simultaneously, recovery orchestration coordinates restoration activities by validating system integrity, synchronising Digital Twin states with physical assets, and progressively returning manufacturing operations to normal conditions while minimising production disruption [18]. Security policies are continuously refined using operational feedback, allowing the defence mechanism to adapt to evolving adversarial tactics and changing manufacturing environments [21].

The adaptive defence cycle follows the sequence

Observe → Predict → Simulate → Evaluate → Mitigate → Learn

where each stage contributes to continuous improvement of cybersecurity performance through iterative feedback and knowledge acquisition [14]. Observed cyber events update the Digital Twin, predictive models estimate attack progression, simulated scenarios evaluate alternative mitigation strategies, and selected responses are implemented automatically before learning mechanisms incorporate operational outcomes into subsequent decision cycles [19]. This closed-loop framework strengthens cyber resilience by enabling intelligent adaptation, reducing response latency, improving recovery effectiveness, and maintaining secure manufacturing operations despite evolving Advanced Persistent Threats [16].

Table 2. Cybersecurity Functions and Digital Twin Intelligence Across Manufacturing Layers

Manufacturing Layer	Digital Twin Intelligence	Primary Cybersecurity Function	Expected Operational Outcome
Physical Manufacturing Layer	Equipment state representation	Asset integrity monitoring	Early detection of equipment compromise
IIoT Layer	Sensor and telemetry fusion	Continuous anomaly detection	Improved operational visibility
Communication Layer	Network state synchronisation	Secure communication monitoring	Reduced network intrusion risk
Digital Twin Layer	Real-time cyber-physical synchronisation	Dynamic situational awareness	Accurate operational representation
AI Analytics Layer	Machine learning, GNNs, Bayesian inference	Threat prediction and attack forecasting	Proactive cyber defence
Threat Intelligence Layer	MITRE ATT&CK, Cyber Kill Chain, behavioural intelligence	Threat correlation and attack attribution	Improved detection accuracy
Decision Support Layer	Risk assessment and asset prioritisation	Intelligent mitigation planning	Faster security decision-making
Security Orchestration Layer	Automated response and continuous learning	Dynamic defence coordination and recovery	Enhanced cyber resilience and operational continuity

4. MATHEMATICAL MODELLING, OPTIMISATION, AND PERFORMANCE EVALUATION FRAMEWORK

4.1 Dynamic Digital Twin State-Space Model

Smart manufacturing systems are characterised by tightly coupled cyber-physical interactions in which operational processes, industrial communication networks, computational resources, and cybersecurity mechanisms evolve simultaneously under dynamic environmental conditions [24]. Conventional state-space models often describe either

physical processes or cyber events independently, thereby overlooking the mutual dependencies that exist between production operations and cybersecurity status [28]. To overcome this limitation, the proposed framework models the Digital Twin as a unified cyber-physical dynamical system capable of continuously representing manufacturing behaviour, network conditions, cyber events, and synchronisation fidelity within a single mathematical formulation. This unified representation enables the Digital Twin to predict future operational states, anticipate evolving attack conditions, and support adaptive cyber defence using continuously acquired telemetry from Industrial Internet of Things (IIoT) devices, industrial controllers, network sensors, and security monitoring platforms [22].

The overall Digital Twin state evolves according to

$$x_{t+1} = A_t x_t + B_t u_t + w_t,$$

where $x_t$denotes the complete cyber-physical system state at time t, $A_t$represents the time-varying system transition matrix, $B_t$describes the influence of defensive control actions, $u_t$denotes mitigation or operational interventions, and $w_t$represents stochastic disturbances arising from process uncertainty, communication variability, equipment failures, or adversarial activities [31].

The complete state vector is expressed as

$$x = \begin{bmatrix} x_c \\ x_p \\ x_n \\ x_d \end{bmatrix},$$

where

- $x_c$represents the cybersecurity state, including intrusion indicators, authentication status, malware activity, and system integrity;
- $x_p$denotes the physical manufacturing state, including machine health, production conditions, equipment utilisation, and process variables;
- $x_n$represents the communication-network state, including bandwidth utilisation, latency, packet loss, routing behaviour, and connectivity; and
- $x_d$denotes the Digital Twin synchronisation state, measuring consistency between physical assets and their virtual counterparts [26].

Unlike conventional monitoring systems that evaluate isolated observations, this coupled state formulation explicitly models interactions among manufacturing operations, communication infrastructure, cybersecurity conditions, and Digital Twin behaviour [23]. Consequently, abnormal changes detected within one subsystem immediately influence estimation of the remaining system states, allowing the framework to recognise coordinated cyber attacks before significant operational disruption occurs [30].

Continuous state estimation is performed through AI inference executed within the Digital Twin, enabling the cybersecurity architecture to forecast future attack conditions, anticipate degradation of manufacturing performance, and evaluate the potential impact of alternative mitigation strategies before their implementation [25]. By continuously updating the cyber-physical state using newly acquired operational observations, the Digital Twin provides a predictive rather than descriptive representation of manufacturing cybersecurity, thereby establishing the mathematical foundation for intelligent attack forecasting and adaptive defence developed in subsequent models [32].

4.2 Multi-stage APT Attack Propagation Model

Advanced Persistent Threats rarely compromise manufacturing environments through a single exploitation event because attackers typically progress through multiple interconnected stages involving reconnaissance, privilege escalation, lateral movement, persistence, credential harvesting, and operational manipulation [29]. Traditional epidemic propagation models assume homogeneous diffusion behaviour and therefore inadequately represent the strategic, targeted, and adaptive nature of modern Advanced Persistent Threats operating within industrial environments [22]. The proposed framework instead models attack progression as a weighted cyber-physical attack graph capable of representing multiple intrusion pathways, infrastructure dependencies, and varying attack probabilities across heterogeneous manufacturing assets [27].

The manufacturing environment is represented as the weighted graph

$$G = (V, E, W),$$

where Vdenotes the collection of cyber-physical assets, including programmable logic controllers, robots, industrial controllers, servers, workstations, cloud services, and network devices; Erepresents feasible attack transitions between interconnected assets; and Wcontains edge weights describing exploitability, communication accessibility, privilege relationships, vulnerability severity, and operational criticality [24]. This graph representation captures the structural relationships that enable attackers to move across manufacturing systems while maintaining persistence and avoiding detection.

Attack progression between infrastructure assets is represented through the attack transition matrix

$$T = [t_{ij}],$$

where each element t_{ij}denotes the probability that an adversary successfully transitions from compromised asset $i$to target asset $j$during a particular attack stage [31]. These transition probabilities may be estimated using Digital Twin simulations, historical cyber incidents, vulnerability assessments, behavioural intelligence, and knowledge derived from frameworks such as MITRE ATT&CK and the Cyber Kill Chain [28]. Because attack probabilities vary according to network topology, system configuration, defensive controls, and attacker capability, the transition matrix evolves dynamically as new operational information becomes available [25].

For every feasible attack path Π, the cumulative compromise probability is expressed as

$$P_{APT} = 1 - \prod_{(i,j)\in\Pi} (1 - t_{ij}),$$

where Πrepresents all feasible attack paths connecting the initial intrusion point to critical manufacturing assets [30]. Rather than analysing attack stages independently, this formulation quantifies the probability that at least one complete attack path succeeds despite the presence of multiple defensive barriers. Consequently, manufacturing assets connected through highly vulnerable pathways receive greater compromise probabilities than isolated or well-protected systems [23].

When integrated with the continuously synchronised Digital Twin, the attack graph supports real-time simulation of adversarial behaviour under changing manufacturing conditions [26]. As vulnerabilities are patched, network configurations change, or defensive actions are implemented, edge weights and transition probabilities are updated automatically, enabling the Digital Twin to generate revised attack forecasts and identify newly emerging compromise pathways [32]. This dynamic graph-based formulation therefore provides a mathematically rigorous foundation for proactive threat prediction, intelligent attack simulation, and adaptive cybersecurity decision-making across smart manufacturing environments [27].

4.3 Dynamic Cyber Risk Optimisation

Cyber risk within smart manufacturing environments is inherently dynamic because the likelihood and consequences of cyber attacks continuously change with production activities, network configurations, asset availability, and defensive interventions [24]. Conventional risk assessment methods frequently estimate cyber risk using static formulations such as probability multiplied by impact and vulnerability, providing only a snapshot of system security without considering temporal evolution or operational constraints [31]. Such approaches are inadequate for Digital Twin-enabled manufacturing environments where cyber threats, production priorities, and mitigation resources evolve simultaneously [27]. The proposed framework therefore formulates cyber risk assessment as a constrained optimisation problem that continuously balances security objectives against operational performance.

The optimisation objective is expressed as

$$\min J = \sum_{t=1}^{T} (w_1 L_t + w_2 C_t + w_3 D_t + w_4 E_t),$$

where $L_t$denotes expected operational loss caused by cyber attacks, $C_t$represents mitigation cost, $D_t$measures production disruption resulting from defensive actions, and $E_t$corresponds to computational expenditure associated with cybersecurity analytics [22]. The weighting coefficients w_1, w_2, w_3, and $w_4$enable decision-makers to prioritise economic performance, operational continuity, cybersecurity effectiveness, or computational efficiency according to organisational objectives [30].

The optimisation is performed subject to computational capacity, response latency, mitigation capability, communication bandwidth, and available cybersecurity resources [25]. Rather than assigning a static numerical risk score, the Digital Twin continuously recalculates the optimal defensive strategy using updated operational telemetry, behavioural intelligence, and predicted attack progression [28]. This formulation enables cybersecurity decisions to adapt dynamically to changing manufacturing conditions while maintaining acceptable operational performance and resource utilisation [32].

4.4 Digital Twin Synchronisation Error

The effectiveness of predictive cybersecurity depends on the ability of the Digital Twin to maintain an accurate representation of the physical manufacturing environment throughout system operation [23]. If synchronisation between physical assets and their virtual counterparts deteriorates, predictions generated by artificial intelligence models become progressively less reliable, reducing the effectiveness of attack forecasting, risk assessment, and automated mitigation [29]. Consequently, synchronisation fidelity represents a critical performance indicator within Digital Twin-enabled cybersecurity architectures.

The synchronisation error is defined as

$$\varepsilon_t = \left\| X_t^{physical} - X_t^{digital} \right\|_2,$$

where $X_t^{physical}$denotes the observed physical manufacturing state and $X_t^{digital}$represents the corresponding Digital Twin state estimated from continuously synchronised operational data [26]. To ensure reliable predictive analysis, the synchronisation error must satisfy

$$\varepsilon_t < \delta,$$

where δrepresents the maximum acceptable synchronisation tolerance determined by application-specific operational requirements [31].

Whenever $\varepsilon_t$approaches or exceeds this threshold, discrepancies between physical and virtual environments may arise because of communication delays, sensor failures, missing telemetry, network congestion, or malicious manipulation of industrial data streams [24]. These discrepancies propagate through artificial intelligence models, reducing attack prediction accuracy, increasing false alarms, and degrading decision confidence [28]. The Digital Twin therefore performs continuous state correction using sensor fusion, redundant observations, and adaptive estimation algorithms to minimise synchronisation error and preserve high-fidelity cyber-physical representation [22]. Maintaining low synchronisation error is essential for ensuring that predictive cybersecurity decisions remain trustworthy throughout changing manufacturing operations [30].

4.5 Adaptive Mitigation Optimisation

Following accurate prediction of cyber threats, an effective cybersecurity architecture must determine which defensive actions should be implemented to maximise risk reduction while operating within practical resource constraints [27]. Because manufacturing organisations possess limited financial resources, computational capacity, and operational flexibility, not every mitigation strategy can be deployed simultaneously [32]. The proposed framework therefore formulates adaptive mitigation as a constrained optimisation problem that selects the combination of defensive actions providing the greatest cybersecurity benefit.

The optimisation objective is expressed as

$$\max \sum_{i} R_i \, a_i,$$

where $a_i$is a binary decision variable indicating whether mitigation strategy $i$is implemented and $R_i$represents the expected reduction in cyber risk achieved by that strategy [23]. Candidate mitigation actions include network isolation, privilege restriction, vulnerability patching, access-control modification, workload migration, endpoint protection, intrusion containment, and system recovery [29].

The optimisation is constrained by the available cybersecurity budget,

$$\sum_{i} c_i \, a_i \leq B,$$

where $c_i$denotes the implementation cost of mitigation strategy $i$and Brepresents the available security budget [25]. Additional operational constraints may incorporate production continuity, maintenance schedules, workforce availability, and regulatory compliance requirements [31].

Within the proposed Digital Twin architecture, mitigation strategies are first evaluated through virtual simulation before deployment to physical manufacturing systems [28]. This capability enables security managers to compare alternative intervention plans, estimate operational consequences, and identify the most cost-effective response without disrupting live production processes [22]. Consequently, adaptive mitigation optimisation strengthens cyber resilience by maximising defensive effectiveness while minimising operational disruption, implementation cost, and unnecessary resource consumption [30].

4.6 Cyber Resilience Index

Measuring the effectiveness of Digital Twin-enabled cybersecurity requires a comprehensive resilience metric that captures not only an organisation's ability to detect and respond to cyber threats but also its capacity to maintain accurate cyber-physical synchronisation and predictive intelligence throughout manufacturing operations [27]. Conventional resilience indicators frequently rely on single performance measures or simple weighted averages, limiting their ability to represent the multidimensional nature of resilience within smart manufacturing environments [29]. To address this limitation, the proposed framework introduces a nonlinear Cyber Resilience Index (CRI) that integrates operational responsiveness, predictive performance, and Digital Twin fidelity into a unified evaluation metric.

The proposed resilience model is defined as

$$CRI = \alpha\left(\frac{MTTD_{ref}}{MTTD}\right) + \beta\left(\frac{MTTR_{ref}}{MTTR}\right) + \gamma P_s + \lambda S_f,$$

where $MTTD$denotes the Mean Time to Detect cyber incidents, $MTTR$represents the Mean Time to Respond, $P_s$is the attack prediction success rate, and $S_f$denotes Digital Twin synchronisation fidelity [24]. The weighting coefficients α, β, γ, and λsatisfy $\alpha + \beta + \gamma + \lambda = 1$, allowing organisations to prioritise operational responsiveness, predictive accuracy, or synchronisation reliability according to strategic objectives [31]. Higher CRI values indicate greater cyber resilience and improved capability to sustain secure manufacturing operations despite evolving Advanced Persistent Threats [22].

4.7 Multi-objective Optimisation

Cybersecurity decisions within smart manufacturing rarely involve a single objective because improving security often increases computational overhead, communication latency, energy consumption, or operational expenditure [30]. Consequently, Digital Twin-enabled cyber defence must balance multiple conflicting objectives simultaneously rather than optimising a single performance indicator [25]. The

proposed framework therefore formulates cybersecurity decision-making as a multi-objective optimisation problem that simultaneously minimises cyber risk while maintaining operational efficiency.

The optimisation problem is expressed as

$$\min\{R\cdot,\ L\cdot atency\ Energy\ Operational\ Cost\},$$

subject to resource capacity, cybersecurity policy, Digital Twin synchronisation, and manufacturing production constraints [28]. Because these objectives are inherently conflicting, no single solution is universally optimal. Instead, Pareto-optimal solutions are generated using algorithms such as the Non-dominated Sorting Genetic Algorithm II (NSGA-II) or Multi-Objective Reinforcement Learning (MORL), enabling decision-makers to select mitigation strategies that best satisfy organisational priorities [32]. By integrating predictive Digital Twin models with multi-objective optimisation, the proposed framework simultaneously enhances cyber resilience, preserves production continuity, reduces operational costs, and supports intelligent real-time cybersecurity decision-making within smart manufacturing environments [26].

5. IMPLEMENTATION CONSIDERATIONS, CHALLENGES AND FUTURE DIRECTIONS

5.1 Practical Deployment Across Smart Manufacturing Environments

The successful implementation of the proposed Digital Twin-enabled cybersecurity architecture requires a carefully planned deployment strategy that accommodates the heterogeneous nature of modern smart manufacturing environments [31]. Most manufacturing facilities continue to operate legacy industrial equipment alongside newly deployed Industrial Internet of Things (IIoT) devices, creating hybrid infrastructures with varying communication protocols, computational capabilities, and cybersecurity requirements [30]. Rather than replacing existing machinery, the proposed framework supports incremental integration through protocol gateways, industrial middleware, and edge computing platforms that enable legacy programmable logic controllers, supervisory control and data acquisition systems, and conventional manufacturing equipment to participate within the Digital Twin ecosystem without disrupting production operations [32].

Edge deployment represents a critical component of the proposed architecture because time-sensitive cybersecurity decisions require local data processing with minimal communication latency [34]. Artificial intelligence inference executed on edge devices enables rapid anomaly detection, attack prediction, and automated mitigation before cyber incidents propagate across production networks. Meanwhile, cloud platforms provide large-scale computational resources for historical data analytics, Digital Twin training, attack simulation, and long-term optimisation while maintaining synchronisation with distributed edge nodes [31]. This edge-cloud collaboration improves scalability by distributing computational workloads according to operational urgency and resource availability.

As manufacturing systems expand, Digital Twin scalability becomes increasingly important. Modular Digital Twin architectures allow additional production lines, robotic systems, and industrial assets to be incorporated without redesigning the cybersecurity framework [33]. Equally important is workforce readiness, as successful deployment depends on engineers and cybersecurity professionals possessing expertise in artificial intelligence, industrial networking, Digital Twin technologies, and cyber-physical system security [34]. Adoption is further strengthened through interoperable communication standards that facilitate seamless information exchange among heterogeneous devices, industrial software platforms, and enterprise management systems, thereby improving operational resilience and long-term maintainability [35].

5.2 Technical, Security, Ethical and Regulatory Challenges

Despite the considerable advantages of Digital Twin-enabled predictive cybersecurity, several technical, ethical, and regulatory challenges must be addressed before widespread industrial adoption can be achieved [36]. Continuous collection of operational telemetry from manufacturing assets introduces significant privacy and data governance concerns, particularly where production information, proprietary process knowledge, or employee activities may be exposed through interconnected Digital Twin platforms [37]. Secure data management policies, encryption mechanisms, and access-control frameworks are therefore essential for protecting sensitive industrial information throughout its lifecycle [38].

Artificial intelligence explainability represents another major challenge because complex deep learning models frequently generate accurate predictions without providing transparent reasoning for cybersecurity decisions [39]. Limited interpretability may reduce operator confidence and complicate forensic investigations following cyber incidents. Furthermore, false-positive detections remain problematic, as excessive security alerts can overwhelm operational personnel, increase response costs, and disrupt manufacturing activities through unnecessary mitigation actions [40]. Continuous model validation, adaptive threshold optimisation, and human-in-the-loop decision support are therefore required to improve predictive reliability.

The computational complexity associated with maintaining continuously synchronised Digital Twins, executing real-time artificial intelligence algorithms, and simulating large-scale attack scenarios may also exceed the processing capabilities of resource-constrained industrial environments [41]. Efficient workload distribution between edge and cloud infrastructures is consequently essential for maintaining acceptable latency

and operational performance [42]. Standardisation remains equally important for ensuring interoperability among industrial systems and cybersecurity platforms. The proposed framework aligns with internationally recognised cybersecurity standards, including IEC 62443 for industrial automation security, the NIST Cybersecurity Framework (NIST CSF) for organisational cyber resilience, and ISO/IEC 27001 for information security management systems, thereby supporting regulatory compliance while promoting secure and trustworthy Digital Twin deployment across manufacturing enterprises [43].

5.3 Future Research Directions and Industrial Implications

Future research should focus on developing increasingly autonomous Digital Twin-enabled cybersecurity systems capable of detecting, predicting, mitigating, and recovering from sophisticated cyber attacks with minimal human intervention [44]. Reinforcement learning, autonomous decision-making, and adaptive security orchestration offer significant opportunities for constructing self-learning cyber defence mechanisms that continuously optimise protection strategies based on evolving operational environments and adversarial behaviour [45]. Similarly, the emergence of Federated Digital Twins will enable geographically distributed manufacturing facilities to exchange cybersecurity intelligence without exposing sensitive operational data, thereby enhancing collaborative threat detection across industrial ecosystems [46].

Rapid advances in quantum computing also necessitate the investigation of quantum-safe cryptographic algorithms capable of protecting future industrial communication networks against quantum-enabled adversaries [47]. Explainable Artificial Intelligence will become increasingly important for improving transparency, regulatory acceptance, and operator trust by providing interpretable explanations for automated cybersecurity decisions [48]. Furthermore, research into self-healing manufacturing systems is expected to transform Digital Twins from passive monitoring platforms into intelligent cyber-physical entities capable of automatically restoring compromised operations following cyber incidents [49]. Extending Digital Twin federation across global manufacturing supply chains would further improve collaborative threat intelligence, coordinated incident response, and cross-organisational cyber resilience, ultimately supporting secure, scalable, and sustainable smart manufacturing ecosystems capable of resisting increasingly sophisticated Advanced Persistent Threats [50].

Table 3. Implementation Challenges, Mitigation Strategies and Future Research Opportunities

Implementation Challenge	Mitigation Strategy	Future Research Opportunity
Integration of legacy manufacturing equipment	Industrial gateways, middleware, protocol translation, phased migration	Universal interoperability frameworks for heterogeneous industrial systems
Limited edge computational resources	Edge-cloud collaborative computing and intelligent workload scheduling	Lightweight AI models and adaptive resource allocation
Digital Twin synchronisation inaccuracies	Real-time sensor fusion, adaptive state estimation, redundant data acquisition	Autonomous synchronisation optimisation using machine learning
Artificial intelligence false positives and limited explainability	Explainable AI, continuous model retraining, human-in-the-loop validation	Trustworthy and transparent industrial AI decision-support systems
Privacy, cybersecurity, and regulatory compliance	Encryption, identity management, zero-trust security architecture, IEC 62443, NIST CSF and ISO/IEC 27001 compliance	Privacy-preserving Digital Twins and federated industrial cybersecurity
Large-scale deployment across manufacturing supply chains	Modular Digital Twin architectures, standardised communication protocols, distributed cybersecurity orchestration	Federated Digital Twins, autonomous cyber defence, quantum-safe industrial cybersecurity, and self-healing manufacturing ecosystems

6. CONCLUSION

This study presented a Digital Twin-enabled cybersecurity architecture for predicting, simulating, and mitigating Advanced Persistent Threats across smart manufacturing systems. By integrating Digital Twins with artificial intelligence, graph-based attack modelling, state-space analysis, constrained optimisation, and adaptive cyber defence, the proposed framework provides a comprehensive approach to enhancing cyber resilience while maintaining operational continuity. The mathematical models developed in this study offer quantitative mechanisms for modelling cyber-physical system dynamics, evaluating attack propagation, optimising mitigation strategies, measuring synchronisation fidelity, and balancing multiple operational objectives. Unlike conventional reactive security approaches, the proposed architecture supports predictive decision-making through

continuous monitoring, real-time simulation, and adaptive learning. The framework also addresses practical deployment considerations, regulatory alignment, and future technological developments, including autonomous cyber defence and federated Digital Twins. Overall, the proposed approach establishes a scalable and analytically rigorous foundation for securing next-generation smart manufacturing environments against increasingly sophisticated and persistent cyber threats while supporting resilient, efficient, and sustainable industrial operations.

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