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Digital twins: State-of-the-art and future directions for modelling and simulation in engineering dynamics applications

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ABSTRACT

This paper presents a review of the state-of-the-art for digital twins in the application domain of engineering dynamics. The focus on applications in dynamics, is because: (i) they offer some of the most challenging aspects of creating an effective digital twin, and (ii) they are relevant to important industrial applications such as energy generation and transport systems. The history of the digital twin is discussed first, along with a review of the associated literature; the process of synthesising a digital twin is then considered, including definition of the aims and objectives of the digital twin. An example of the asset management phase for a wind turbine is included in order to demonstrate how the synthesis process might be applied in practice. In order to illustrate modelling issues arising in the construction of a digital twin, a detailed case study is presented, based on a physical twin which is a small-scale three-storey structure. This case study shows the progression towards a digital twin highlighting key processes including: system identification, data-augmented modelling and verification and validation. Finally, a discussion of some open research problems and technological challenges is given, including: workflow, joints, uncertainty management and the quantification of trust. In a companion paper, as part of this special issue, a mathematical framework for digital twin applications is developed, and together the authors believe this represents a firm framework for developing digital twin applications in the area of engineering dynamics.

23 1 Introduction

24 Society is experiencing an era of *digital transformation*. It is now common to hear concepts discussed in the technical
25 literature and wider media relating to this transition. Concepts such as *Industry 4.0*, *the Internet-of-Things* [1], and *Big*
26 *Data* [2], amongst others, have become increasingly widely used, particularly in relation to engineering applications. Often
27 mentioned in this context, and promoted as a potentially transformative idea for engineers working in all areas, is the idea of
28 a *digital twin*. In this paper, the focus will be on modelling and simulation, and in this context, a digital twin can be defined
29 as a virtual duplicate of a system built from a fusion of models and data. This is made possible by combining models *and*
30 data using state-of-the-art algorithms, expert knowledge and digital connectivity. The potential benefit of the digital twin is
31 a significant improvement in predictive capability compared with current technologies.

32 Like all areas of modern endeavour, the vast majority of engineering applications are becoming increasingly reliant on
33 computing – for example, creating numerical simulations that are used to inform decisions about the design and management
34 of key components, structures, and systems. In the last few decades, high-performance computing (HPC) has been employed
35 extensively to build increasingly high-fidelity models in the belief that this would remove *model form* uncertainties associated
36 with the engineering application being considered. Whilst this has given considerable benefit, there are still a large number
37 of engineering problems with high levels of uncertainty even after the application of HPC [3], and this serves to dispel the
38 idea that increasing levels of model fidelity is a panacea, although it is undoubtedly helpful in many situations. As a result,
39 obtaining a useful virtual model is no longer a question of increasing model fidelity, but now rests in the more difficult
40 problem of developing *trust* (or conversely dealing with the remaining uncertainties) in the model(s) through other means.

41 An important technical example where this situation occurs is in the problem of modelling mechanical joints. The
42 physics associated with mechanical joints is still the subject of considerable research, and as a result, physics-based models
43 are subject to considerable epistemic uncertainty. One reason for this situation is that many of the physical processes happen
44 at the tribological scale (microns), whereas the modelling of the whole joint, and the rest of the structural behaviour, is
45 required at much larger (macro) scales. Common phenomena like friction and hysteresis are difficult to model for the same
46 reason. In addition, systems operating in dynamic environments are often highly sensitive to very small disturbances to the
47 structure (typically assumed to be aleatory uncertainties). In the case of joints for example, small differences in tolerances,
48 and other joint properties, such as friction, are highly sensitive to temperature variations in the operating environment, which
49 can all lead to large deviations in the dynamic behaviour of a jointed structure. From a modelling perspective, it is very
50 difficult to bring together models of all these different physical processes, and their associated uncertainties, which happen
51 at different length scales, into an accurate model of a complete structure, even when large amounts of computing power are
52 available.

53 In parallel, an organisational example of the problems faced in creating effective simulations of modern engineering
54 applications occurs in the way problems are analysed, designed and simulated as subsystems. This is a natural approach
55 because most modern engineering systems are highly complex, and as a result, it makes sense to have multiple teams of
56 experts carrying out computations of the subsystems in parallel. However, once this type of division is made, there is a
57 natural tendency for the teams to work in *silos*. This silo effect, combined with the fact that the subsystems are often defined
58 based on the different physics or scales involved, means that the resulting subsystem models often cannot be unified into a
59 model of the complete application. This mixing of technical objectives with inappropriate organisational culture can lead to
60 undesirable outcomes such as *analysis paralysis* [4], amongst others.

61 The main transformative aspect of the digital twin is to improve predictive capability by augmenting computational
62 models using data; this again reflects the wider digital transformations happening in society. Analysis of data, particularly
63 through internet and social media applications, has been a very important modern phenomenon. For example, techniques
64 such as machine learning are now used in order to provide bespoke targeting of consumer behaviour, such as advertising
65 and other related activities. In engineering, advancements in sensor technology mean that many systems now have the
66 potential to gather and process *very* large amounts of data. Structures are increasingly being built with sensors embedded,
67 and this combined with advances in structural health monitoring (SHM) and associated *data-based* techniques, means that
68 the potential to exploit information obtained from data is rapidly increasing [5].

69 For the purposes of the applications considered here, the main idea of the digital twin is to combine these model-based
70 and data-based approaches to create a virtual prediction tool that can evolve over time. In doing so, the digital twin concept
71 offers the potential to assist in engineering applications for both technical and organisational problems, such as the two
72 examples mentioned above. In the technical example, the main idea would be to reduce the epistemic uncertainties from
73 the limitations of the physics-based modelling, using data. These data would be obtained from the real structure, which is
74 called the *physical twin*, or laboratory tests using components from the structure – in either case, it is important that the data
75 gathered are specific to the structure being twinned, as the digital twin is *entirely bespoke* to this structure. To address the
76 organisational example, the digital twin concept incorporates a hierarchical format, enabling multi-scale and multi-physics
77 processes to be incorporated, but most importantly a highly connected organisational framework that should offer solutions to
78 the problem of silos, and related cultural issues. The digital twin approach also seeks to break down unhelpful organisational
79 barriers (i.e. improve connectivity) by providing a logical interface of outputs and inputs from different computational models
80 (in different silos), ideally by using robust *Verification & Validation* (V&V) methods that build trust in the subsystems prior

81 to the assembly of these into a full system digital twin.

82 In terms of maturity, the digital twin is a relatively new idea, one that has attracted significant attention in many areas of
83 engineering and beyond; it offers a range of highly-attractive potential solutions to engineers who are tasked with designing
84 and managing ever more complex engineering systems. However, there are substantial challenges to be overcome in order
85 for digital twin technology to reach full maturity.

86 The aims of this paper are twofold; firstly, it is to assess the current state-of-the-art of digital twins when applied
87 to engineering systems with time-dependent (i.e. dynamic) behaviour; secondly, is to summarise the outstanding open
88 research problems and technological challenges. The reason for focusing on applications in dynamics is that: (i) they
89 offer some of the most challenging aspects of creating an effective digital twin, and (ii) they are relevant to important
90 industrial applications such as energy generation and transport systems. In a companion paper, as part of this special issue,
91 a mathematical framework for digital twin applications is developed, and together the authors believe this represents a firm
92 framework for developing digital twin applications in the area of engineering dynamics.

93 The paper is structured as follows. In Section 2 the background to, and history of, the digital twin will be discussed,
94 including examples of the current state-of-the-art in engineering dynamics. In Section 3 the process of synthesising a digital
95 twin is discussed in detail. Then, in Section 5, an example of a simulation digital twin for the asset management phase of
96 a wind turbine structure is presented. In Section 6, a case study of a digital twin of a small-scale three-storey building is
97 presented, in order to demonstrate how a selection of model and data-based algorithms can be unified into the digital twin.
98 After that, open research problems and technological challenges are discussed in Section 7, before the conclusions are given
99 in Section 8.

100 2 History and background to the digital twin

101 The origins of the twinning concept have been attributed by some authors [6], to the work of NASA during the Apollo
102 programme. The term *digital twin* appears to have developed from work relating to product lifecycle management (see [7]
103 and references therein), although other names were being used for similar concepts in other domains at around the same
104 time, for example *digital counterpart* [8], *virtual engine* [9] or *intelligent prognostics tool* [10], amongst others [11]. The
105 term digital twin captured the zeitgeist and as a result is now typically taken as a generic term to encompass all these
106 related phrases, although, as previously stated above, the meaning relies heavily on the specific context involved. The idea
107 has received considerable attention since then in the area of product design, with particular overlap with existing digital
108 design tools such as computer-aided-design (CAD) [12, 13], big data and data-driven design [14–17], knowledge graphs and
109 relations to ontologies [18, 19], middleware [20, 21] and blockchain [22].

110 The concept has also been considered extensively in the domain of manufacturing processes, including autonomous
111 manufacturing [6, 11], real-time manufacturing [23], computer-aided design [24, 25], additive manufacturing [26, 27] and
112 more general innovations in manufacturing processes including links to cyber-physical systems [28–40].

113 In terms of asset management, digital twins have been considered for tasks such as damage detection and structural-
114 health/condition monitoring [10, 28, 41] and uncertainty quantification [42]. In addition to the application areas already
115 mentioned, digital twins have also been considered for application in the areas of offshore drilling [43], offshore wind
116 turbines [44, 45], space structures [46] and nuclear fusion [47].

117 An important consideration for the concept is, how the digital twin relates to the life-cycle of the product or process in
118 question [48]. The majority of applications cited above are applied to manage the performance of an engineering application
119 after its design and manufacture, but a digital twin would ideally be delivered with the product at the start of its operational
120 life, and would also capture all aspects of the manufacturing process [3]. Therefore, whenever possible, the digital twin
121 would need to be first implemented during the *design phase*, and persist throughout the entire operational life of the product
122 (which is called the *asset management phase*) [49]. In both lifecycle phases, valuable information may be provided by
123 data or models aggregated from similar structures, or even from the wider population. It is anticipated that for engineering
124 applications, one of the most important high-level objectives that a digital twin can be used for is structural life prediction.
125 Examples including the current state-of-the-art in engineering dynamics are considered next.

126 2.1 Structural life prediction using a digital twin

127 In 2011, Tuegel *et al.* proposed a new way of estimating the life of an aircraft [3]. The authors imagined a future
128 scenario where every new aircraft was delivered with a digital twin. The digital twin would represent the real aircraft (the
129 physical twin) so closely that it could, for example, include the effects of manufacturing anomalies, and details of the material
130 micro-structure. As a result the digital twin could be used to give ultra-realistic predictions about the life of the aircraft.

131 Of course, this vision of ultra-high fidelity modelling has been a long-held ambition in many industrial design sectors.
132 The example put forward by Tuegel *et al.* was distinguished, not only because it proposed the digital twin as a solution, but
133 also because it articulated some of the key challenges to achieving this vision.

134 There are three important problems that Tuegel *et al.* [3] describe that are common for a wide range of engineering

135 applications. The first problem is that of multi-scale modelling – called by some *the tyranny of scales* [50]. This term refers
136 to the problem of modelling the behaviour of physical phenomena that display radically different, dominant behaviours at
137 different length scales. This issue is also closely linked to the problem of dealing with different types of physical modelling at
138 different scales (or domains), and creating effective interfaces between them – often given the catch-all label of *multi-physics*
139 *modelling*. The second problem Tuegel *et al.* identified is the *gap between hardware capability and software performance*,
140 something recognised in the HPC research community, and a major factor in limiting the ability of engineers to harness the
141 full benefit of increasing amounts of computing power. The third problem is that of *historical processes* during the design
142 stage, with the result that the historical nature of the process is a restriction to progress.

143 In particular, digital computing has been applied to design and analysis to make computations faster, more efficient, and
144 of higher resolution than previously possible; but often the design process is still based on the pre-digital computer methods.
145 Furthermore, rather than offering more freedom to designers of complex engineering systems, the rapid advancement of
146 computational methods has meant that designers are increasingly locked into existing processes. This situation is often,
147 in large part, because of the necessity to do many parts of the design in parallel. Typically large teams of engineers will
148 work on just one part of the overall system. This practice often creates silos, that as the computational methods become
149 increasingly sophisticated, become so deeply engrained, that any form of integration with other parts of the design process
150 becomes extremely difficult.

151 Furthermore, the pursuit of a digital twin will involve improving physics-based modelling techniques. A key area of
152 improvement will be geometry adaptation and morphing throughout the life of the structure. This may be required in order
153 to capture behaviours due to manufacturing anomalies as stated by Tuegel *et al.* [3]. The ability to have CAD representations
154 that are a one-to-one mapping of the physical twin will be necessary for certain models. In addition, with multiple models
155 integrated to generate a digital twin, links such as joint models will play a vital role. Joints pose a major challenge because
156 a large portion of modelling difficulties will come from subsystem interactions. Solutions to these problems may not lie
157 completely in physics-based modelling itself. Data augmentation may provide an additional avenue for correcting physics-
158 based models, so that they more closely reflect the physical twin. This crucial ‘building block’ interacts with all others, and
159 will be discussed further in the following sections.

160 2.2 Verification and validation using digital twins

161 For engineering dynamics there is a well-established set of techniques for *Verification and Validation* (V&V). More
162 specifically, as most dynamics applications are assumed to have linear dynamics, *modal analysis & testing* has become the
163 de facto method for validation against measured data – see for example [51] and references therein. This methodology makes
164 a direct connection between the model(s) and the measured data using the concept of *modes of vibration*. In fact, the methods
165 have been extended so that operational modal analysis can be applied using only response data recorded from the structure
166 under normal operation conditions [52]. More generally the vibration modes can be interpreted in both a physics-based
167 model context (typically a finite element model representing the geometric and material properties of the system) and as an
168 identification technique (or data-based model).

169 A more general framework for verification and validation processes encompasses the concepts of white, grey and black-
170 box models [53, 54]. Starting from the assumption that a model can be built with physics-based reasoning, then the object
171 of interest is called a ‘white-box model’. At the other end of the spectrum, ‘black-box’ models are derived entirely from
172 measured data, with no assumed knowledge of the physics at all. In between these two extremes, grey-box models are a
173 combination of both physics-based reasoning and data. This combination of models and data is exactly the format required
174 for a digital twin. That said, it is natural to ask; what is the difference between the digital twin and a validated model? The
175 answer will be context specific, but a digital twin will typically be time-evolving and make much more extensive use of
176 data [3].

177 In structural dynamics and other branches of computational mechanics, there have been many previous advancements
178 in this area. For example, finite element updating methods adjust model parameters based on experimental observations,
179 in order to match the model parameters to the measured experimental system [55]. This type of *model updating* will need
180 to be a key functionality of the digital twin, with frequent updates, ultimately in near real-time, creating the time-evolving
181 property required of the twin. This would provide a mechanism for performing structural health monitoring and would aid
182 asset management decision making. In combination with updating, the digital twin can make use of a range of data-based
183 algorithms; e.g. to carry out condition monitoring of the structure, based on an evolving history of measured data. Already,
184 machine learning methods are proving to be some of the most productive algorithms used for this purpose [5, 56], and this
185 will continue to develop as a key part of digital twin technology, see for example [57, 58].

186 In recent years, a number of application-specific guidelines have been proposed for implementing the model validation
187 process (verification is discussed in Section 5.3). For example, one of the first such frameworks to focus on physics-based
188 engineering models was that produced in 1999 by the AIAA for computational fluid dynamics (CFD) problems [59]. These
189 frontrunners have been followed more recently by a series of standards introduced by the American Society of Mechanical
190 Engineers (ASME), currently comprising the ASME Guide for V&V in Computational Solid Mechanics in 2006 [60] and the

191 Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer in 2009 [61]. These documents
192 provide a firm basis for the application of validation methods, and many aspects of these frameworks can be transferred to
193 dynamic problems. However, validation of nonlinear dynamical models presents additional challenges that are yet to be
194 fully addressed, and an issue of particular interest is how to account for potential bifurcations in the response of a nonlinear
195 system.

196 3 Synthesising a digital twin

197 As discussed in the previous Section, validated models and process control are both natural starting point for synthe-
198 sising a digital twin. Of course, the digital twin is much more than just a validated model or a control process. In this
199 context, a digital twin needs to be a robustly-validated, time-evolving virtual duplicate of the physical twin that aids decision
200 making. Ideally the digital twin would be synthesised during the design phase, and continue to evolve during manufacture,
201 commissioning, operation and finally decommissioning.

202 3.1 Process control and condition monitoring

203 It is important to note that some aspects of the digital twin concept have evolved from condition monitoring of plant, or
204 supervision of other processes (i.e. process control). At a most basic level, *supervision* is the first desirable aim; beyond this,
205 many industrial plant and asset management systems have highly-developed operational capabilities. This type of interactive
206 capability represents the second category, which will be called *operational*, meaning that the operational decisions are
207 informed and supported by relevant information. Both supervision and operational capabilities are long established, and
208 although some authors mention these as digital twins, here they are considered to be *pre-digital twins*, meaning a system
209 that has the capability to be a digital twin but currently does not contain all the essential elements (where essential elements
210 means those elements that give the required functionalities required of a digital twin, which in this paper are taken to be;
211 simulation; learning and management).

212 The next level of sophistication is that described by Tuegel *et al.* [3], and is categorised as a *simulation digital twin*. It is
213 important to note that this typically incorporates both supervision and operation into its processes as well as simulation. In
214 this sense, it builds on and enhances the pre-digital twin capabilities by adding the ability to simulate, based on models and
215 data, the physical twin. This type of digital twin will also be able to allow the user to visualise a graphical interpretation of
216 the physical twin, and carry out predictions to support design or operational decisions. As stated in the Introduction, here a
217 key requirement of a simulation digital twin is that it should be able to provide the user with a quantitative assessment of the
218 level of trust (via uncertainty quantification) for each simulation or prediction it produces.

219 Building on the concept of a simulation digital twin (or *simulation twin*) are two more levels of sophistication, both of
220 which are currently aspirations for the digital twin. The first advance is to add an increased degree of ‘intelligence’ to the
221 digital twin, to give an *intelligent digital twin*. This object includes all the capabilities of the simulation twin, adds the ability
222 to learn from data (via machine learning) and also adds increased levels of decision support and scenario planning.

223 The final level of sophistication is the digital twin that allows the physical twin to be autonomous. As before, the
224 digital twin would include all previous capabilities, and add the ability for the twin to carry out all decision making (within
225 prescribed parameters) and manage the asset concerned with minimal human intervention. There is also the possibility
226 of adding higher levels of learning and intelligence capabilities, via artificial intelligence techniques, although this is not
227 discussed here.

228 The hierarchy of possible capabilities is shown in Fig. 1.

229 A key distinguishing feature of a digital twin (and hence the dividing line between Levels 2 and 3 in Fig. 1) is that it can
230 be used as a predictive tool. A process control interpretation naturally relates to asset management tasks, but aims for the
231 twin can also be defined in the design phase, as will be discussed later in Section 4.1.

232 4 Context specific aim and objectives of a digital twin

233 For nearly all applications, the primary aim of creating a digital twin is to enable the user to have as much information
234 as possible about the current status and future behaviour of the physical twin, such that optimal decisions can be made. The
235 precise objectives of the digital twin will depend on the context that is required, but a typical simulation twin for a dynamics
236 application might allow the user to:

- 237 1 quickly understand the outputs with fast (possibly real-time if required) visualisation of results;
- 238 2 incorporate and update the geometry of the digital twin through integrated computer-aided-design (CAD);
- 239 3 navigate through the CAD model to specific components or sub-assemblies of interest and perform isolated tasks;
- 240 4 identify spurious behaviour, potential damage or the need for system maintenance;
- 241 5 view a hierarchical representation of physical behaviour at different length scales;
- 242 6 interrogate the current state of the structure, whether in real-time or historically, and perform data analysis (diagnosis);

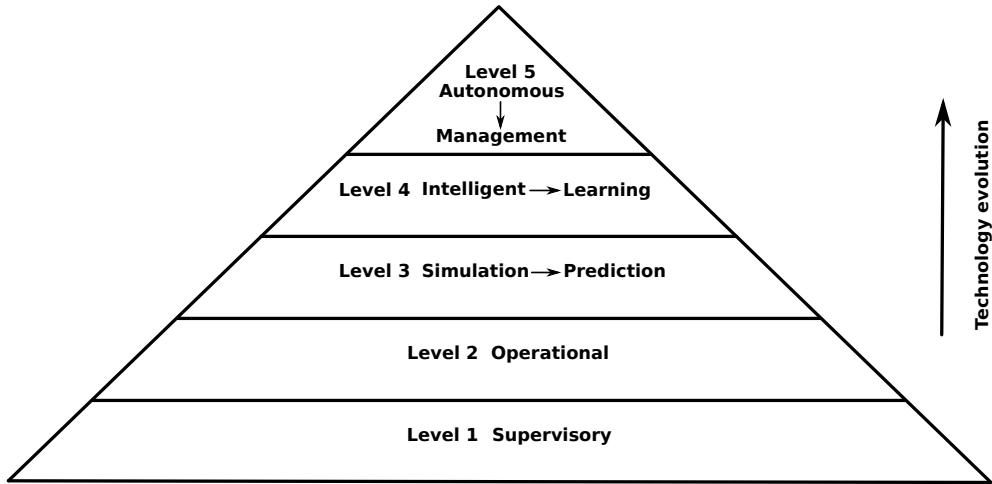


Fig. 1: A capabilities hierarchy for digital twins, where each level incorporates all the previous capabilities of the levels below

- 243 7 simulate future scenarios to make predictions (prognosis & decision support);
- 244 8 design controllers, perform hardware-in-the-loop simulation and/or set control processes for the physical twin;
- 245 9 quantify a level of confidence (trust) that can be given to simulation outputs.

246 Note that the abilities to predict future outcomes, and quantify the level of confidence in these predictions are particularly
 247 important features. The synthesis of a simulation digital twin during first the design, and then the asset management phases,
 248 is now considered.

249 4.1 Digital twins during the product design phase

250 The design phase is considered first here, as envisaged, for example, by Tuegel *et al.* [3], where a new product (an
 251 aircraft in the case cited) is delivered to the customer with a digital twin that can then be used for asset management. Design
 252 processes are also context dependent, and for the broad context of dynamics applications a typical standpoint is to use the
 253 ‘Design V’ model as shown in Fig. 2, that emphasises the role of verification and validation during the design manufacture
 254 and commissioning.

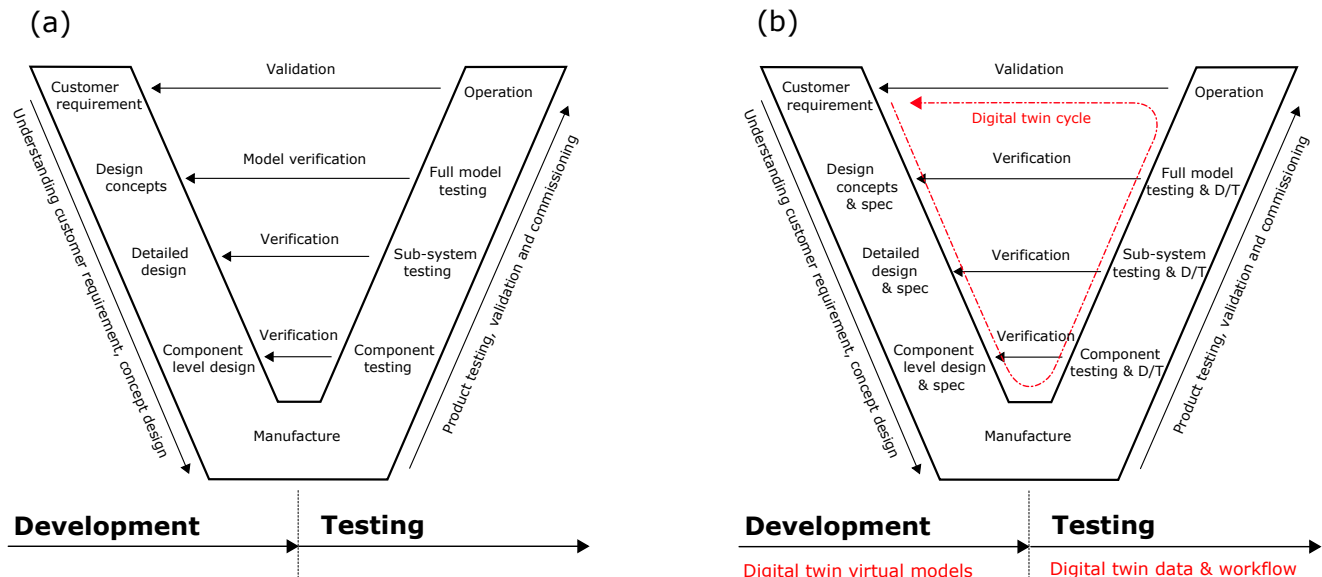


Fig. 2: Schematic representation of the V model for product design. (a) The traditional V model, and (b) the V model with a digital twin cycle added. Note that D/T is shorthand notation for digital twin, and P/T is shorthand notation for physical twin

255 Fig. 2 (a) shows the traditional V model, where starting at the top left with customer requirements, the design is first
 256 developed going down the left-hand part of the V to manufacture. The product is then verified and validated as the process
 257 continues up the right-hand side of the V until commissioning is complete. In this context, verifying is checking that all the
 258 tasks in the process are carried out correctly (Fig. 3: Did we build the thing right?), and validation is checking to see that
 259 the final product delivers the required overall performance (Fig. 3: Did we we build the right thing?). Fig. 2 (b) shows how
 260 the V model can be modified to include a digital twin cycle. In this scenario, the verification and validation process is used
 261 to build a digital twin, starting with component-level testing data, and progressing to subsystem and finally full (or as full as
 262 possible), system tests. Note also, that a new step can be included for a first stage validation of the digital twin, shown in
 263 Fig. 2 (b) as the culmination of the digital twin cycle. This is a first stage validation, because the digital twin will need to be
 264 regularly re-validated through-out its life, in order to ensure that it can continue to deliver highly trusted outputs.
 265 As the digital twin is a combination of models and data, the first stage of the cycle shown in Fig. 2 (b) is the development
 266 of physics-based models through the detailed design phase. These models are then augmented with data collected from the
 267 product testing and commissioning phase to build a product-specific digital twin. A specific example of this type of data
 268 augmentation process will be given in Section 5.5.

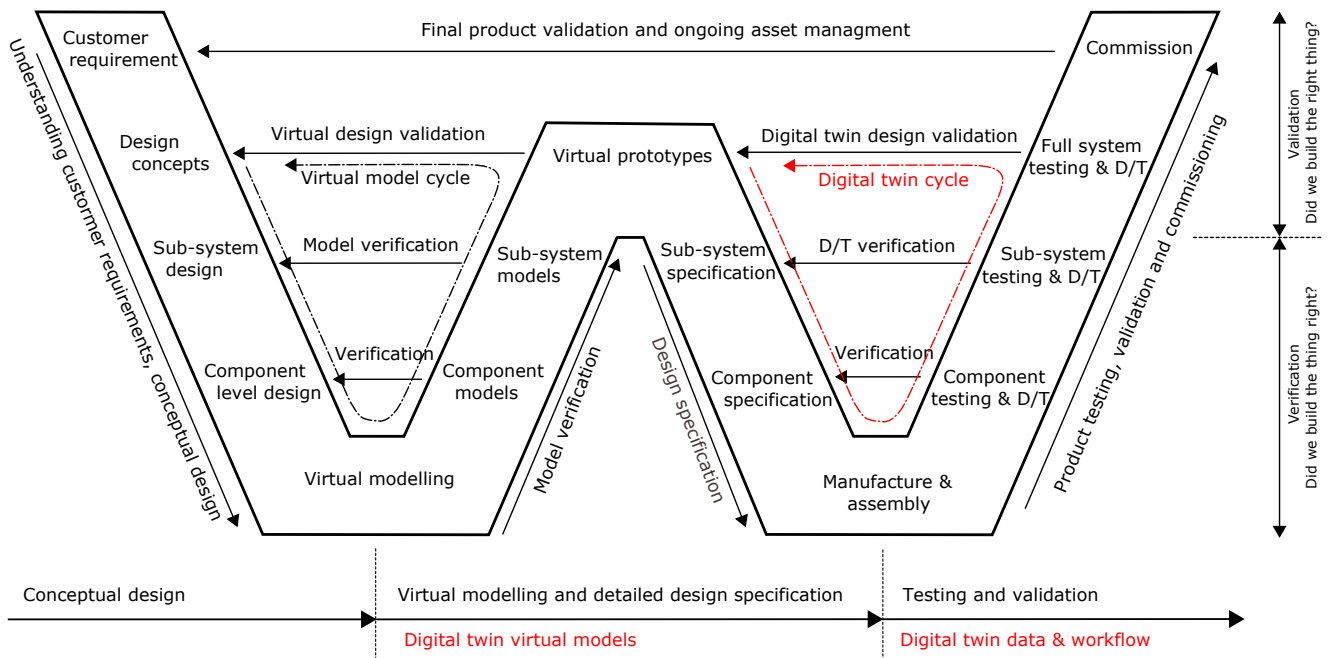


Fig. 3: Schematic representation of the W model for product design. In this case a specific virtual prototyping stage is included. The virtual prototype is then used as the basis for a digital twin in the second cycle

269 To be more specific, the initial design phase can be separated from the virtual modelling and commissioning phases,
 270 as shown schematically in Fig. 3, where the model now resembles a W. In this case, a specific virtual prototyping stage
 271 is included that precedes the testing and validation phase. The virtual prototypes then form the basis for synthesising the
 272 digital twin in the second part of the cycle. Note that the idea of a W model has been previously proposed in the context of software
 273 engineering [62–64]. The concept is somewhat different from the idea proposed here. For example in [62] the W model
 274 defines one V for the component development process, whilst the other V is for the system development process, and these
 275 two V's are integrated into a single overall method.

276 In this context, the primary aim of the digital twin is to reduce uncertainties by incorporating component/subsystem
 277 data, and where possible, shorten the testing and validation phase for the full system based on the assumed reduction in
 278 uncertainty. Another important consideration is how the digital twin will transfer into the asset management phase, and this
 279 is discussed next.

280 4.2 Digital twins during the asset management phase

281 Assuming the digital twin has already been synthesised during the design phase, it then needs to be extended into the
 282 asset management phase. To do this, the required digital twin capability level is first selected, typically levels 3,4 or 5, as
 283 shown in Fig. 1. Then, depending on the context and the required functionality, the *essential elements* are selected, based on

284 the required aim and objectives of the digital twin. For the selected essential elements, a matrix of building blocks can be
 285 created, and a representative example is shown in Fig. 4, that for the purposes of giving insight, includes all the capability
 286 levels from Fig. 1.

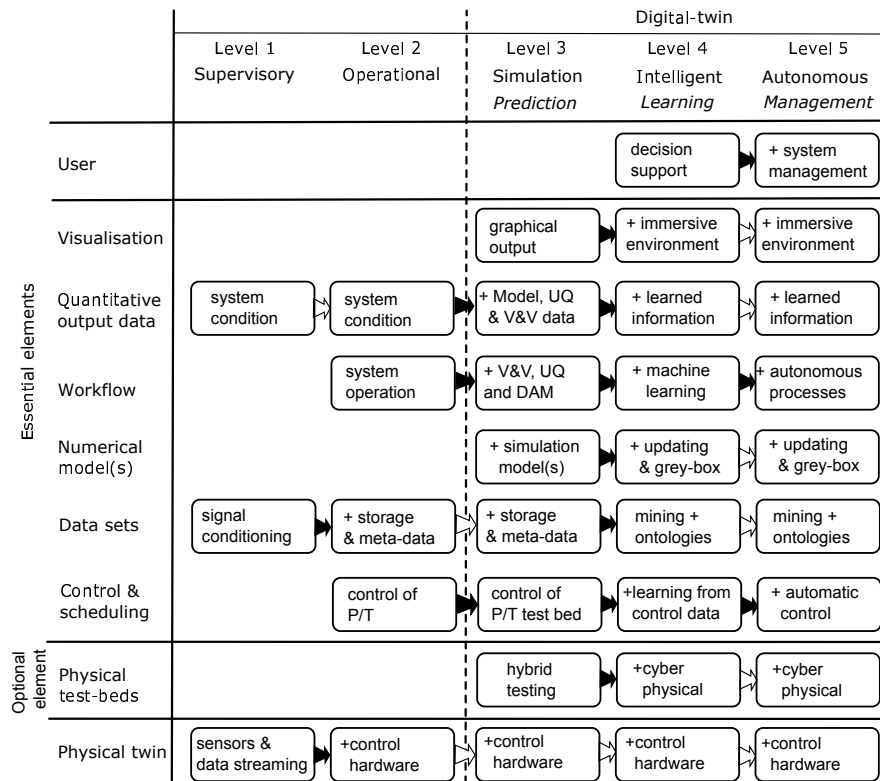


Fig. 4: Schematic representation of the building blocks required for the five levels of digital twin. Note that only a selection of the possible process building blocks are shown in the workflow. Moving from left to right each block incorporates the functionality of the previous block. Solid black arrows indicate new functionality, and white arrows indicate no new functionality. P/T is physical twin, V & V is verification and validation

287 Here it can be seen that the pre-digital twins do not contain all the essential elements required for a digital twin; neither
 288 do they have the key distinguishing features of a digital twin, namely the ability to predict, learn and manage. Within the
 289 matrix, individual building blocks are shown, although it should be noted that these are indicative rather than prescriptive.
 290 The exact requirements will depend on the precise context. Note also that only a selection of the possible process building
 291 blocks are shown in the workflow.

292 The capability levels in Fig. 4 increase from left to right. Furthermore, moving from left to right, each building block
 293 incorporates the functionality of the previous block. Solid black arrows indicate that a new functionality has been added,
 294 while white arrows indicate no new functionality. Again this arrangement should be regarded as indicative rather than
 295 prescriptive, as specific choices will be made by the digital twin designer. For example, moving from Level 3 to Level 4
 296 in the Numerical Models element adds model updating and grey-box modelling capability in Fig. 4, indicating an increase
 297 in sophistication of the new level. It should be noted however, that changes between levels will be dependent on the exact
 298 context of the digital twin.

299 An important distinction is made between Level 3, and Levels 4 and 5, with regards to the user. In Level 3, it is assumed
 300 that the user is responsible for all the ‘cognitive’ tasks, such as deciding which workflow processes to run, making decisions,
 301 and the overall management of the physical twin. At Levels 4 and 5 some of these tasks are anticipated to be incorporated
 302 into the digital twin functionality. This matter is a key area of future development for digital twin technology. The discussion
 303 is now extended further by using the example of a simulation digital twin.

304 **5 Example elements of simulation digital twin**

305 As an example, a simulation twin for the asset management phase of a wind turbine, is determined from the matrix in
 306 Fig. 4. A schematic representation of the simulation digital twin is shown in Fig. 5.

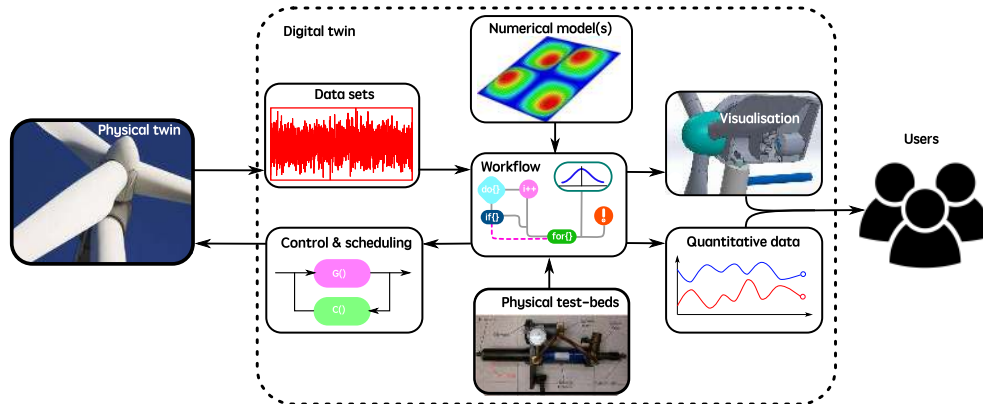


Fig. 5: Schematic representation of a simulation digital twin during an asset management phase, showing the essential elements for the simulation twin and their interrelations

307 Here, data sets are recorded from the physical twin, and control and scheduling commands fed back as required (enabling
 308 supervision and operation). The recorded data (potentially in real-time and from similar or legacy sources) are used for tasks
 309 in combination with the numerical model(s) and physical test bed(s) (which can include further online devices, systems or
 310 databases) to give the required simulation capability. The interaction of these different elements is coordinated by a *workflow*,
 311 which also provides the user with visualisation and quantitative feedback.

312 The concept of workflow is well established in the domain of software engineering [65–69] and business process man-
 313 agement [70]. Several authors have considered the problem of verifying the soundness of workflows, for example [71–73].

314 In the context of this current work, the role of the workflow is to deliver and coordinate all the *required processes* that
 315 the digital twin is expected to perform. There must also be a user interface enabling commands to be received by the digital
 316 twin and also to provide quantitative and visual feedback. Once the commands are received, the workflow will coordinate
 317 and sequence the required processes, based on the aims and objectives of the digital twin. The required processes themselves
 318 can be built from relevant algorithms coordinated within the workflow (these algorithms can be aligned to the building blocks
 319 shown in Fig. 5).

320 The example considered here is of a simulation twin requiring *uncertainty quantification* (UQ), and so it shall be assumed
 321 that the required algorithms are:

- 322 1 physics-based modelling;
- 323 2 software integration and management;
- 324 3 verification & validation;
- 325 4 uncertainty quantification;
- 326 5 data-augmented modelling;
- 327 6 output visualisation.

328 In addition to a workflow process related to each building block, it is possible that additional workflow processes can
 329 be created by combining and further augmenting these underlying building blocks. For the current example of a simulation
 330 twin, each of the separate building blocks listed above are now discussed briefly.

331 **5.1 Physics-based modelling**

332 Physics-based modelling is a well-established field within engineering. In essence, it is the process of using knowledge
 333 about physics, based on experimental observations, in order to construct mathematical representations of the system of
 334 interest. This takes many forms in engineering, from first-principles models, to approximation-based techniques such as
 335 finite element analysis (FEA), computational fluid dynamics (CFD) and multi-body physics models. Of course, a key starting
 336 point in the development of many digital twins will be the generation of physics-based models (which will be formed from
 337 expert elicitation).

338 It is important to recognise that, despite the application of large amounts of computing power, the vast majority of
 339 engineering applications do not have a single ultra-high fidelity model that captures all possible physics; this is because

340 it is typically impossible to simultaneously replicate the behaviour of all the physical processes happening, at all scales
341 for anything except the most simple applications. As a result, engineers typically use multiple models, capturing different
342 physical processes, at different length scales, and with a range of fidelities, for the same system. The essence of the digital
343 twin concept is that these models can be augmented with available data, and beyond that with each other (a process that
344 overlaps with existing techniques of model verification [74]). The primary purpose of this data and model augmentation is
345 to increase the confidence in the prediction being made with the physics-based model.

346 Within the workflow, two other important processes are required of the physics-based models. The first deals with
347 combining multiple models of the structure into the complete digital twin. Typically, companies will produce multiple
348 models of the structure. This normally occurs due to the department divisions within an organisation, due to expertise or the
349 design process. These models will capture different physics, be modelled at different fidelities, and be at different scales e.g.
350 component, sub-assemblies. As a result, new opportunities for validating the complete digital twin occur; whereby these
351 validated component or subsystem models are used to provide an understanding of the validity of the (full system) digital
352 twin. By combining multiple models, the workflow provides significant gains on the current concepts of isolated validated
353 models.

354 The second scenario occurs when specific models for particular tasks are needed at a particular level of efficiency. For
355 example, a high-fidelity FEA model may be constructed, but may be too computationally expensive to run for an online
356 fatigue estimation task for a hotspot of interest (although with the increase in computational power this may become a less
357 frequent problem). Instead a bespoke, more efficient, model may be generated from the FEA model for this task; this could
358 be a reduced-order model, as commonly utilised in dynamics applications, or could be an efficient surrogate or emulator of
359 a complex computer model [75, 76].

360 5.2 Software integration and management

361 The set of physics-based models utilised as part of a digital twin will need managing and integrating. The variety of
362 solvers, software providers, and outputs will all require interactions with a main user interface (and potentially with each
363 other) via workflows; the question is how might this be achieved? One possible solution is that the digital twin workflow will
364 coordinate, and call as required, other software packages or bespoke pieces of code to perform required subtasks – this is
365 called *loose coupling* by [3], as opposed to using a single solver for all the physical processes, which is called *tight coupling*.
366 In this sense, the workflow would operate (at least in part) as a ‘wrapper’ with a user interface. Multiple existing subtasks can
367 then be run in parallel, or cross-coupled to create new *super-tasks*, some of which may not have been previously achievable.

368 However, linking pieces of proprietary software together is fraught with its own set of difficulties. In addition to this,
369 writing bespoke pieces of code for each application could be considered inefficient in the long term. Several authors have
370 suggested using the concept of *blockchains* for digital twins, based on open source code [22, 34]. It has been suggested that
371 blockchains could be used to implement a range of different features, based on a clearly-defined software architecture, for
372 example a ‘visual program’ interface, that enables users to connect ‘programming blocks’ together to obtain the required
373 functionality. However, it seems that that the blockchain concept has evolved more toward secure transaction applications,
374 which may not be so relevant in engineering, except where there is overlap with connected business processes. Whatever
375 software architecture is used, the workflow will need to encode a series of logical steps in each process (for example [71]),
376 in order to capture the sophisticated level of task coordination required.

377 Key to any implementation, is effective representation of coupled physical processes, either through multi-physics mod-
378 elling or coupling software/simulation codes to capture the required behaviour; this will often be made more challenging due
379 to large differences in temporal and spatial scales.

380 5.3 Verification & Validation

381 Verification is defined by Oberkampf and Roy as ‘the process of determining that the numerical algorithms are correctly
382 implemented in the computer code and of identifying errors in the software’ [74]. The subject is divided into subcategories
383 of software quality assurance (SQA) and *algorithm verification*, where SQA relates to checking the interactions of code
384 as part of a wider software, and algorithm verification is interested in the correctness of the implementation of particular
385 mathematical formulae. These two categories must both be implemented and used for a digital twin to be realised, as in
386 practice, fundamental verification will be expected as part of employing any commercial software. Here, the particular chal-
387 lenges in verifying the software integration and management strategies described in Section 5.2 (part of SQA) are discussed.
388 Moreover, an outline of the verification (algorithm verification) of machine learning and black-box approaches that may be
389 incorporated as part of data-augmented modelling is given.

390 A fundamental task of a digital twin is to perform predictions. To gain any confidence in these predictions, validation
391 must be conducted. The process of validating a model requires: (i) quantitatively measuring the accuracy of the model output
392 against experimental data, (ii) providing a measure of confidence in the predictions, both when interpolating or extrapolating,
393 in the models intended context of use, (iii) determining whether the accuracy of the model is appropriate for the intended
394 use [77]. In the context of a digital twin this becomes the process of validating several models, with different outputs, where

395 (as previously mentioned) the tyranny of scales applies. Consequently, validation must be considered at a system level in
396 combination with the sub-model level. Moreover, it is argued that a digital twin cannot be fully realised without incorporating
397 the quantification and propagation of uncertainties. As a result, validation processes and metrics will need to accommodate
398 these uncertainties.

399 In order to perform validation, data sets must be obtained. Obtaining data sets is a particular challenge for many full-
400 system structures. It may be possible to obtain data for one time instance, but impossible to acquire data for all possible
401 outcomes a user may wish to model or for multiple repeats. The validation process therefore needs to be conducted for parts
402 of the digital twin where data are obtainable.

403 5.4 Uncertainty quantification

404 The aspiration of a digital twin is: a close one-to-one mapping between a physical and virtual system, which is only
405 achievable through acknowledging uncertainties involved in both physical observations and computer models. A classifica-
406 tion of these uncertainties, outlined by Kennedy and O’Hagan [75], follows:

- 407 - *Parameter uncertainties* – computer models inevitably contain parameters which may be measurable (in which case
408 there is parametric variability) but in most cases are not fully known or accessible.
- 409 - *Model discrepancy* – following the famous quote by Box [78] that ‘All models are wrong but some are useful’, it is
410 understood that even when the parameters are deterministic and ‘truly’ known (in an engineering context this will occur
411 when the parameters have physical meaning), there will still be mismatches between the model output and the ‘true’
412 physical process (without observational uncertainty).
- 413 - *Residual variability* - given the same set of inputs the process may produce different outputs, due to a chaotic (due to
414 not knowing the inputs to the required accuracy) or stochastic nature. This is often a problem with the inputs not being
415 sufficiently detailed.
- 416 - *Parametric variability* – the situation in which the model is utilised may vary because inputs cannot be fully controlled
417 or specified. A model may however require a specification of a single deterministic value, which should be varied based
418 on knowledge of the process.
- 419 - *Observational uncertainty* – measuring any real world structure will result in a level of measurement error or noise.
- 420 - *Code uncertainty* – most computer models are sufficiently complex that the output from a model is unknown until it is
421 evaluated. An approach commonly utilised within surrogate modelling is therefore to treat it as uncertain at locations
422 where the computer model has not yet been evaluated.

423 The task of uncertainty quantification (UQ) in a general context is to provide a measure of these sources of uncertainty,
424 often jointly, in order to reflect the overall level of uncertainty inherent in both the model predictions and the gathered data. It
425 is common practice to subsequently propagate the identified uncertainties through the model in order to evaluate variability in
426 the predicted quantities of interest. Comparison of these predictions with experimental data over some appropriately specified
427 validation domain lies at the heart of model validation, discussed in Section 5.3. The core processes involved in uncertainty
428 quantification are model selection and parameter estimation (in different contexts, referred to as system identification or
429 model updating). The processes of quantifying uncertainty in parameters may be achieved via a variety of approaches.
430 Linear and non-linear regression are widely used in a frequentist context, but make an assumption that parameters are fixed
431 but unknown and offer a limited characterisation of parameter distributions. Bayesian methods [79] have proven hugely
432 popular in recent years with application of Markov Chain Monte Carlo (MCMC) methods (e.g. the Metropolis Hastings
433 algorithm [80]) being key to their practical application. Such techniques offer the possibility of building a detailed description
434 of the distributions of uncertain model parameters at the cost of being computationally demanding; computational cost
435 concerns for challenging distributions are addressed to some extent through developments of the basic MCMC algorithm
436 (e.g. Transitional MCMC [81]). With regard to model selection, and the errors that will inevitably occur as a result of
437 the computational model not being able to perfectly reflect the underlying physics of the modelled process, there are two
438 principle schools of thought. The effect of model form error/discrepancy is typically handled through a choice to either
439 subsume this error within the parameter estimates, potentially biasing them (something of particular concern in cases where
440 the parameters have physical meaning); or to explicitly model the discrepancy as considered in Section 5.5. The tradeoff
441 between these approaches is considered in more detail in [82].

442 In a digital twin context, the uncertainty quantification process may involve application of techniques from the general
443 toolbox of methods for UQ to multiple contributing models. The process is complicated by the fact that system-level
444 predictions may be the result of result of multiple, interacting sub-models. If there is coupling between these models (for
445 example the bidirectional coupling typically required in multi-physics or multi-scale model; or in multi-level models where
446 parameters at one level form states at another level [83]), the complexity of the UQ task grows substantially. Further,
447 decision making on the basis of multiple, uncertain model outputs is a substantially more complex task than for a single
448 model. Ensemble forecasting, where weightings are applied in a principled fashion to the predictions of multiple generating
449 models, offers a potential direction of travel in this area [84].

450 Finally, a key distinguishing feature of a digital twin is their evolution over time. The implication here is that any
451 uncertainty quantification technique may need to operate in, or close to, real time – a major constraint on many current
452 technologies. Achieving real-time (or near real-time) UQ for a digital twin may require the development of highly computa-
453 tionally efficient estimation techniques [85]; the adoption of fast-running statistical surrogates that approximate the response
454 of the underlying computational models within the digital twin [86, 87]; or periodic updating when differences between the
455 physical and digital twin outputs are deemed to have occurred.

456 5.5 Data-augmented modelling

457 It is never possible to fully capture all possible physics affecting a structure within a computer model, regardless of
458 the level of fidelity. Consequently, a digital twin cannot be formulated solely from the outputs of physics-based computer
459 models if the aim is to achieve ultra-realistic predictions. As outlined in the uncertainty quantification section, this problem
460 is captured by the model discrepancy term. Using the knowledge that computer modelling alone will provide inadequate
461 solutions to generating a digital twin, models must be augmented using information available from data in order to improve
462 predictive capabilities.

463 One approach to data-augmented modelling assumes that a computer model can be embodied as [75],

$$464 \mathbf{z}(\mathbf{x}) = \mathbf{y}(\mathbf{x}) + e = \boldsymbol{\eta}(\mathbf{x}, \boldsymbol{\theta}) + \boldsymbol{\delta}(\mathbf{x}) + e \quad (1)$$

464 where $\mathbf{z}(\mathbf{x})$ are the observations of the system outputs $\mathbf{y}(\mathbf{x})$, which are subject to uncertainties represented by the error term
465 e . The bias (or model discrepancy)-corrected computer model outputs $\mathbf{y}(\mathbf{x})$ are functions of the inputs \mathbf{x} . Equation 1 states
466 that $\mathbf{y}(\mathbf{x})$ is equal to the sum of the computer model $\boldsymbol{\eta}(\mathbf{x}, \boldsymbol{\theta})$ and the model discrepancy $\boldsymbol{\delta}(\mathbf{x})$, where the $\boldsymbol{\theta}$ are parameters of
467 the computer model.

468 Equation 1 provides a framework for utilising additive machine learning methods in order to infer the model discrepancy
469 and noise process. Without acknowledgement that model discrepancy exists and parameters inferred during uncertainty
470 quantification will be biased and/or overconfident, which will lead to inaccurate predictions [88]. More generally, grey-
471 box modelling — the combination of a white box (a physics-based model) and a black box (from machine learning or a
472 statistical process) — encompasses the range of approaches whereby machine learning methods are inserted into physical
473 model structures such that unknown physics can be accounted for and inferred from data.

474 5.6 Output visualisation

475 Digital twins will organise a vast amount of information, most of which will be processed through well-established
476 visualisation techniques. In addition, new methods of data visualisation will become possible. Notably, augmented/virtual
477 reality or augmented/virtual inspection, as proposed by Moreu *et al.* [89] are expected to become more prevalent. By having
478 a one-to-one mapping in the virtual domain, inspection tools can be combined in real time with the outputs of the digital
479 twin, to guide and inform inspectors.

480 6 Case study: Towards a digital twin of a small scale three-storey building

481 In order to illustrate the philosophy of moving from pre-digital-twins to a digital-twin, specifically one incorporating
482 elements of levels 3 and 4 of a digital twin, a three-storey structure is introduced as a case study. In this scenario, the
483 experimental test structure is taken to be the physical twin with the asset management objective being to construct a digital
484 twin that can predict and monitor the accelerations at each of the three storeys.

485 In between the top two floors of the physical twin is a ‘bumper’ mechanism — two aluminium blocks, where one is
486 attached to the top floor and the other to the middle floor. When specific excitation and initial conditions are met, the two
487 blocks come into contact, introducing a harsh nonlinearity. This nonlinearity provides a demonstration of when traditional
488 approaches to generating a validated model may fail. As a result, technologies are presented that move towards the aspiration
489 of a digital twin.

490 In this case study, a scenario is imagined in which the structure is designed to operate under a random excitation applied
491 at the first floor at a consistent forcing level. In the design and construction phase of the physical twin it is assumed that
492 the ‘bumper’ mechanism will not come into contact, and therefore the system is treated as linear in the initial modelling
493 stage. This was decided as under initial testing there was no activation of the ‘bumper’ mechanism. This reflects common
494 decisions made within industry, where often due to modelling difficulties, computational capacity and prior assumptions a
495 simplified (often linear) computer model is generated, as long as it provides adequate predictive performance. Once in the
496 operational phase and under the same band-limited white noise forcing level, the ‘bumper’ mechanism of the physical twin
497 is shown to occasionally introduce the harsh nonlinearity. The case study therefore reflects common real world scenarios
498 whereby unforeseen behaviour occurs from the physical twin, and the digital twin is expected to replicate or at least inform

499 the operators of these events. This case study therefore presents some of the challenges and technologies required in creating
 500 a digital twin.

501 6.1 Experimental setup and data gathering

502 The physical twin is illustrated in Fig. 6 and has three storeys. Each floor is constructed from an aluminium block with
 503 a mass of 5.2 kg and dimensions $350 \times 255 \times 5$ mm ($L \times w \times h$). The floors are joined by vertical columns, with each column
 504 having a mass of 55 g and dimensions $555 \times 25 \times 1.5$ mm. The blocks used to connect the columns to the floors have a mass
 505 of 18 g and dimensions $25 \times 25 \times 13$ mm. For each of these connections, four Viraj A2-70 grade bolts were used with a mass
 of 10 g each.

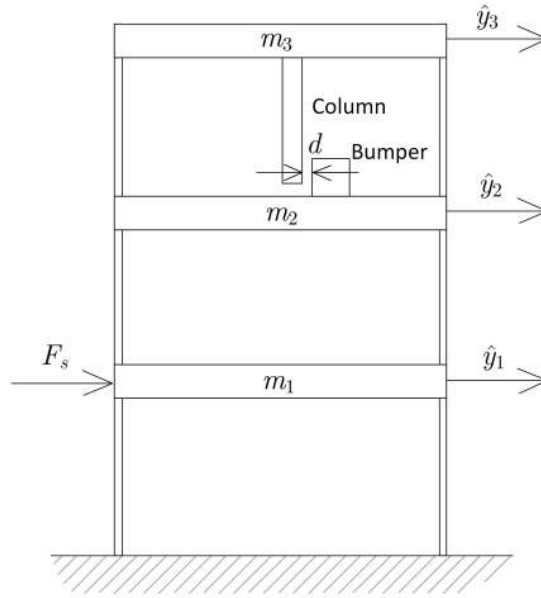


Fig. 6: The three storey structure physical twin — a schematic diagram detailing the shaker attachment and accelerometer positioning

506 The system is excited by a shaker attached at the first floor and a transducer is used to measure the force applied by the
 507 shaker. The experimental data were acquired using an LMS CADA system connected to a SCADAS-3 interface. Data were
 508 recorded at a sampling frequency of 51.2 Hz using piezoelectric accelerometers fixed to each storey as shown in Fig. 6. The
 509 structure was consistently excited with a 25.6 Hz band-limited white noise source at the same excitation level.

510 Three data sets were collected. Each of the three data sets were 20-second observations of the structure under the
 511 random excitation source. In the first two data sets, used as a training and testing set in the following analyses, the ‘bumper’
 512 mechanism did not come into contact. The third data set is a scenario in which there was contact in the ‘bumper’
 513 mechanism.

514 6.2 Initial Modelling: System identification

515 Although the physical twin is ultimately a nonlinear system, the initial data from the physical twin in operation did not
 516 include any contact in the ‘bumper’ mechanism. For this reason the initial modelling stage assumed a linear model with
 517 which to perform system identification. Frequency response functions (FRFs) for the system, shown in Fig. 7, indicate that a
 518 three-degree-of-freedom model of the physical twin should be sufficient to capture the main dynamics of the structure. The
 519 proposed model is given by,

$$\begin{aligned}
 \ddot{y}_1 &= (F_s - k_1 y_1 - k_2(y_1 - y_2) - c_1 \dot{y}_1 - c_2(\dot{y}_1 - \dot{y}_2))/m_1 \\
 \ddot{y}_2 &= (k_2(y_1 - y_2) - k_3(y_2 - y_3) + c_2(\dot{y}_1 - \dot{y}_2) - c_3(\dot{y}_2 - \dot{y}_3))/m_2 \\
 \ddot{y}_3 &= (k_3(y_2 - y_3) + c_3(\dot{y}_2 - \dot{y}_3))/m_3
 \end{aligned} \tag{2}$$

520 where $\{m_i\}_{i=1:3}$ are the masses, $\{c_i\}_{i=1:3}$ are the damping coefficients and $\{k_i\}_{i=1:3}$ are the stiffness coefficients for each
 521 of the three floors (indexed by i). Additionally the force, displacement, velocity and acceleration terms are denoted as F_s ,
 522 $\{y_i\}_{i=1:3}$, $\{\dot{y}_i\}_{i=1:3}$ and $\{\ddot{y}_i\}_{i=1:3}$ respectively. The physics-based model selected here is analytical, however the principles
 523 and techniques discussed are applicable to more complex model forms, such as finite element or multi-physics models.

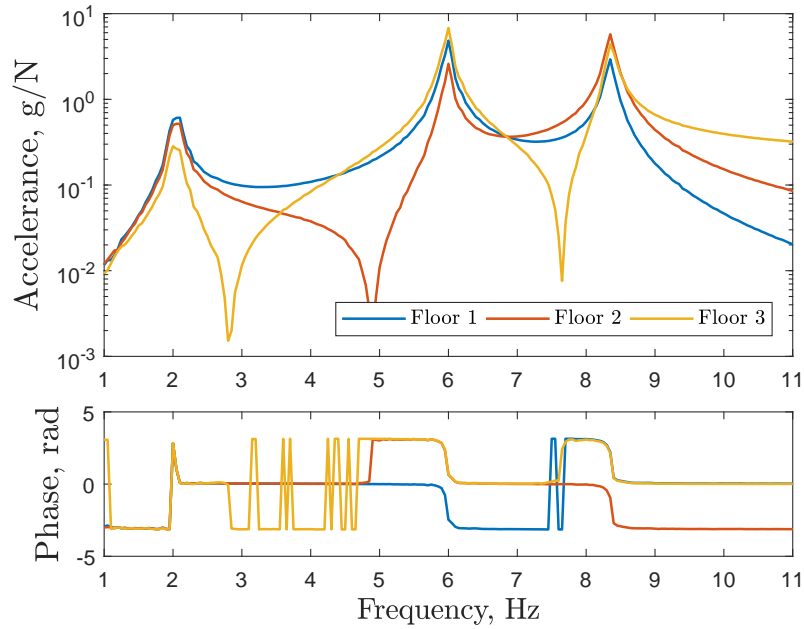


Fig. 7: FRFs between the first floor and the accelerations from each of the three floors

s

524 Parameters for this model were identified using the *Self Adaptive Differential Evolution* (SADE) algorithm. For full
 525 details of this algorithm, the reader is referred to the original paper [90]; for details of how it is implemented as an identifi-
 526 cation method, see [91, 92]. Briefly, as in all evolutionary optimisation procedures, a population of possible solutions (here,
 527 the vector of parameter estimates), is iterated in such a way that succeeding generations of the population contain better
 528 solutions to the problem in accordance with the Darwinian principle of survival of the fittest. The problem is framed here
 529 as a minimisation problem with the cost function defined as a normalised mean-square error (NMSE) between the measured
 530 data and that predicted using a given parameter estimate,

$$J_i(\theta) = \frac{100}{N\sigma_{\ddot{y}_i}^2} \sum_{i=1}^N (\ddot{y}_i - \hat{\ddot{y}}_i(\theta))^2 \quad (3)$$

531 where $\sigma_{\ddot{y}_i}^2$ is the variance of the measured sequence of relative accelerations and the caret denotes a predicted quantity; N is
 532 the number of ‘training’ points used for identification, and θ is the parameter. The total cost function J was then taken as the
 533 average of the J_i . Previous experience has shown that a cost value of less than 5.0 represents a good set of model predictions
 534 (or parameter estimates). In order to generate the predictions $\hat{\ddot{y}}_i$, the coupled equations (2) were integrated forward in time
 535 in Matlab using a fixed-step fourth-order Runge-Kutta scheme for initial value problems. The excitations for the predictions
 536 were established by using the measured forces. The SADE identification scheme is computationally expensive, with the
 537 main overhead associated with integrating trial equations forward in time. For this reason, the training set (or identification
 538 set) used here was composed of only $N = 400$ points. To avoid problems associated with transients, the cost function was
 539 only evaluated from the final 200 points of each predicted record. The first of the four data sets where the physical twin
 540 exhibited linear behaviour is used as the training data set.

541 The SADE algorithm was initialised with a population of randomly-selected parameter vectors or individuals. The
 542 parameters were generated using uniform distributions on specified initial ranges. The initial ranges (estimated based on
 543 engineering judgement) were [4.5, 7] for the masses, [0, 6] for the damping and $[0, 2 \times 10^5]$ for the stiffness. A population of
 544 200 individuals was chosen for the SADE runs with a maximum number of generations of 100. In order to sample different
 545 random initial conditions for the DE algorithm, 10 independent runs were made. Each of the 10 runs of the DE algorithm

Table 1: Parameter estimates from 10 independent SADE runs

Parameter	Best	Maximum	Minimum	Mean	Standard Deviation	Coefficient of Variation
m_1	4.864	4.887	4.501	4.763	0.140	0.029
m_2	5.353	6.884	5.353	5.976	0.443	0.074
m_3	5.380	6.304	5.380	5.840	0.262	0.045
c_1	4.541	6.000	3.242	4.913	1.010	0.206
c_2	0.000	0.083	0.000	0.011	0.027	2.418
c_3	0.000	1.172	0.000	0.349	0.461	1.323
$k_1 (\times 10^3)$	4.100	4.425	2.887	4.012	0.505	0.126
$k_2 (\times 10^3)$	4.146	4.768	4.058	4.303	0.212	0.049
$k_3 (\times 10^3)$	4.906	6.134	4.906	5.467	0.347	0.064
J	1.620	2.457	1.620	2.042	0.307	0.150

546 converged to a good solution to the problem in the sense that cost function values of around 2% or below were obtained in all
 547 cases; the summary results are given in Table 1. The best solution gave a cost function value of 1.620. A visual comparison
 548 of the ‘true’ experimental responses for an unseen test data set (the second data set where the ‘bumper’ mechanism did not
 549 make contact) and the predicted response given the best parameter set is given in Fig. 8.

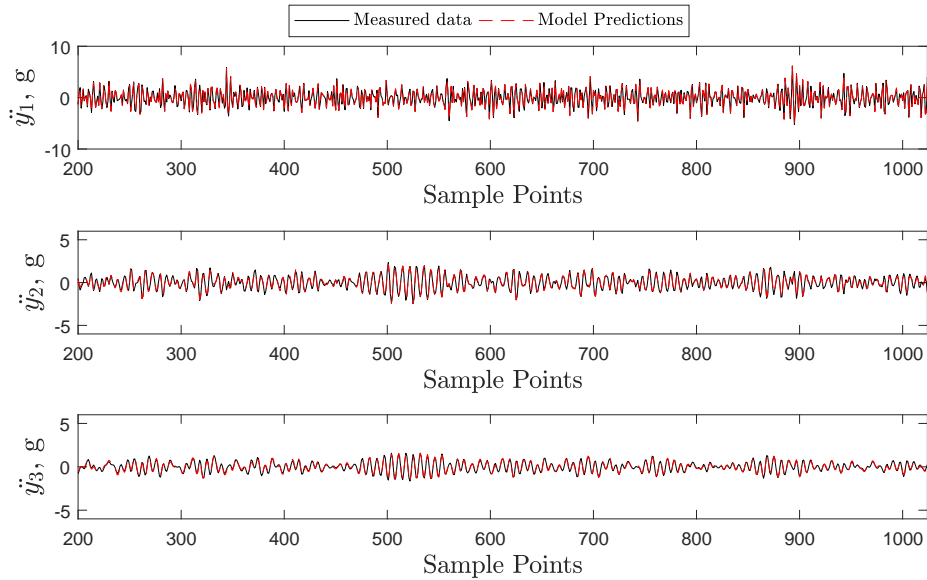


Fig. 8: SADE model predictions on testing data (no ‘bumper’ contact)

550 These results show that the objective of the digital twin has been met. Based on the validation metric (NMSE) the
 551 digital twin is shown to have good performance on the test set. Traditionally this digital twin would then be expect to operate
 552 for the duration of the structure’s life. The process shown here compares to industry norms, in which a model may be
 553 deterministically calibrated and validated and expected to predict the structure performance. However, the calibrated model
 554 is then applied to the third data set, in which the ‘bumper’ mechanism comes into contact, introducing a harsh nonlinearity.
 555 Predictions of the digital twin in this region fail as presented in Fig. 9. The NMSE for these predictions are 20.644, 55.724
 556 and 34.421 for the acceleration at each floor. This is compared to, 0.317, 1.640 and 1.928 on the training data set and 0.417,
 557 2.877 and 3.778 on the test data set. The shows that the model has failed in its objective of predicting the accelerations at

558 each floor in the new context.

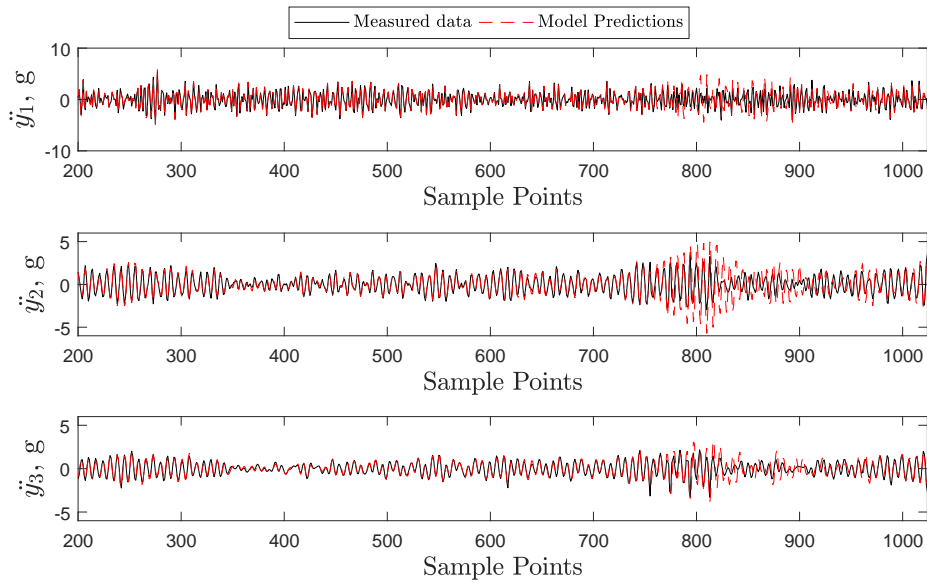


Fig. 9: SADE model predictions on validation data ('bumper' contact)

559 6.3 Uncertainty Quantification

560 Moving towards level three of a digital twin means incorporating knowledge about the uncertainty in the system. Given
561 the same physical model and training, testing and validation data sets, Bayesian calibration (or system identification) was
562 performed. By incorporating uncertainty estimation within the workflow allows the extraction of more information about the
563 performance of the digital twin.

564 In this case study Markov Chain Monte Carlo (MCMC) — using the Metropolis Hastings algorithm — was used to
565 perform Bayesian inference for the same linear analytical model (Equation 2). A joint Gaussian likelihood (the product of
566 the Gaussian likelihood for each floor) was used, where the noise variance was fixed ($\sigma^2 = 3 \times 10^{-3}$) reflecting engineering
567 judgement of the sensors. Gaussian priors were also formulated for the mass, stiffness and damping coefficients where the
568 mean for each prior was the best fit from the SADE analysis (shown in Table 1), with variances of $\sigma^2 = 10$ for the mass and
569 damping coefficients and 1×10^8 for the stiffness coefficients. Four MCMC chains were run in parallel with random start
570 locations and the \hat{R} statistics measured to check convergence. As Bayesian parameter estimation is not the topic of this paper
571 the reader is referred to [80, 82] for more details on MCMC for uncertainty quantification.

572 Four independent MCMC chains were run all initialised at different random initial conditions. 10000 samples were
573 obtained with a burn-in of period of 2500 samples. The \hat{R} statistics were checked for all the parameters. It was found that
574 although the chains had satisfactorily converged, the likelihood was relatively insensitive to the damping coefficients. Every
575 twentieth sample was taken from the first chain, this is performed in order to protect against any residual autocorrelation
576 in the chains. The estimate parameter distributions from the MCMC analysis are shown in Fig. 10. It can be seen that the
577 values estimated by SADE (Table 1) are all within the estimated distributions apart from the first damping term c_1 . This again
578 shows the difficulty of estimating damping, due to the relative insensitivities in the acceleration in a lightly damped metallic
579 structure — confirmed by the high coefficient of variation in the SADE estimates. This shows the information gained about
580 the structure from uncertainty quantification.

581 The output predictions for these samples are shown on the testing (no 'bumper' contact) and validation ('bumper'
582 contact) sets in Figs. 11 and 12. These figures illustrate good predictive performance for the test data set; however, as
583 expected, they fail to predict the validation set. The histogram of the NMSEs for the outputs from the parameter samples are
584 shown in Fig. 13, stating that the model performs well on the test data and fails on the validation data. The figure also shows
585 that the SADE NMSE results are at the lower end of the histograms.

586 6.4 Data augmented modelling

587 An additional step in moving towards a digital twin is to augment the model with data. Here a Gaussian Process model
588 is used to infer model discrepancies for the predicted output from the linear model. This is the equivalent of performing

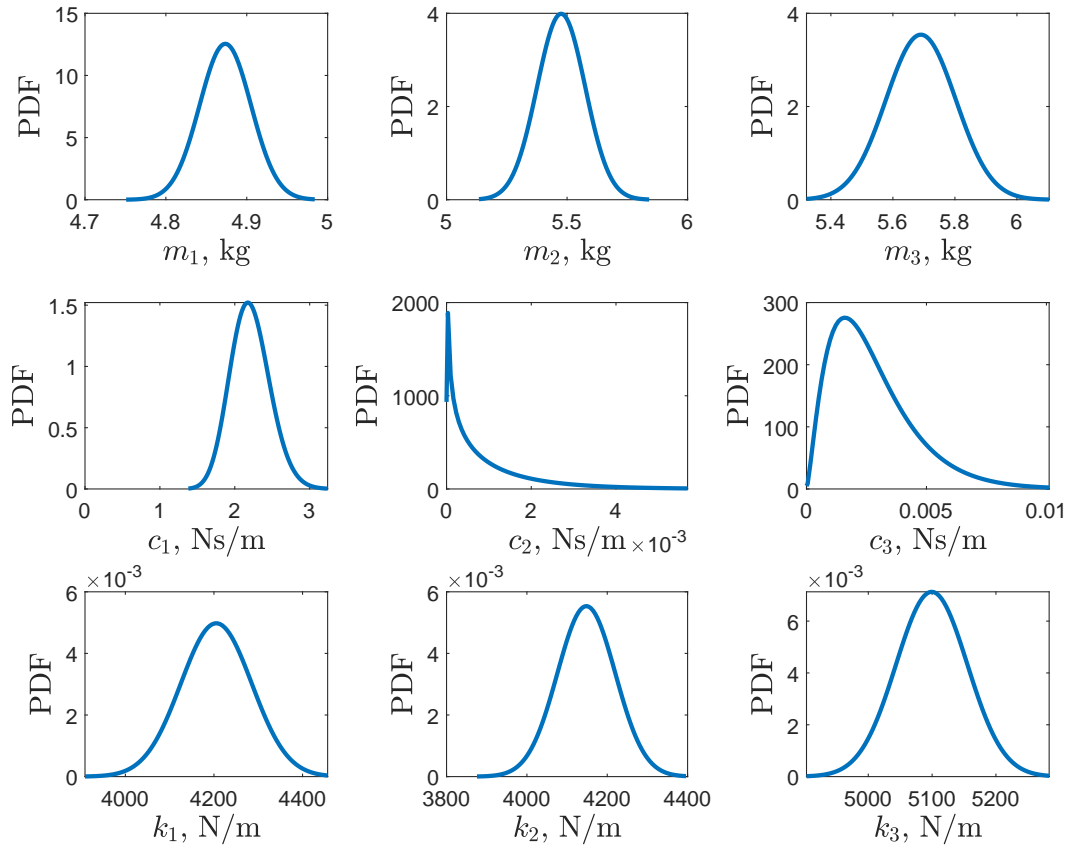


Fig. 10: MCMC parameter distributions

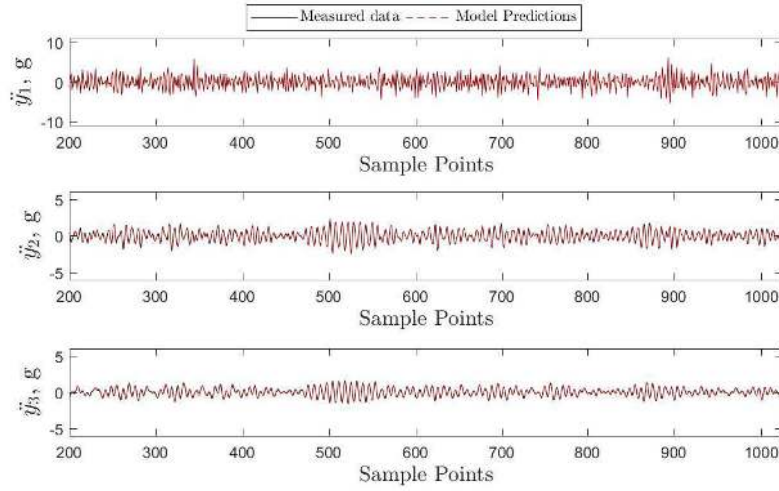


Fig. 11: MCMC model predictions on testing data (no 'bumper' contact)

589 equation 1 in two stages, i.e. a parameter inference step to determine the parameters θ of the computer model $\eta(\vec{x}, \vec{\theta})$ and
 590 then a discrepancy step to infer $\delta(\mathbf{x}) + e$.

591 The discrepancies are believed to contain dynamic information and for this reason the inputs to the Gaussian process
 592 (GP) model are lagged outputs of the linear model and the input forcing (where the forcing is expected to be known at time t_n
 593 as it is measured) i.e. $\{\dots, \ddot{y}_i(t_n - 3), \ddot{y}_i(t_n - 2), \ddot{y}_i(t_n - 1), \dots, \ddot{F}(t_n - 3), \ddot{F}(t_n - 2), \ddot{F}(t_n - 1), \ddot{F}(t_n)\}$; where the outputs from
 594 the linear model are the averaged output prediction from the MCMC samples. This type of model is equivalent to $\delta(\mathbf{x}, \dot{\mathbf{y}}) + e$.
 595 To determine the number of lags used within the data-augmented model the autocorrelation of the residual between the linear
 596 model predictions and training observations were calculated. This informed that there was correlation up to around ten lags,

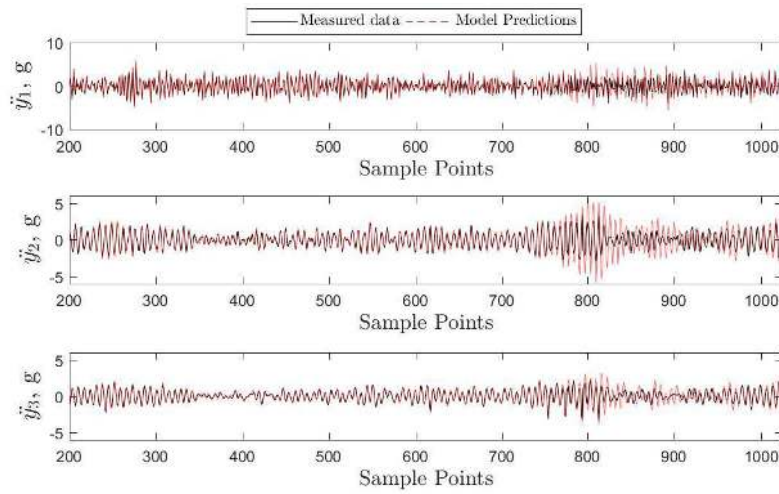


Fig. 12: MCMC model predictions on validation data ('bumper' contact)

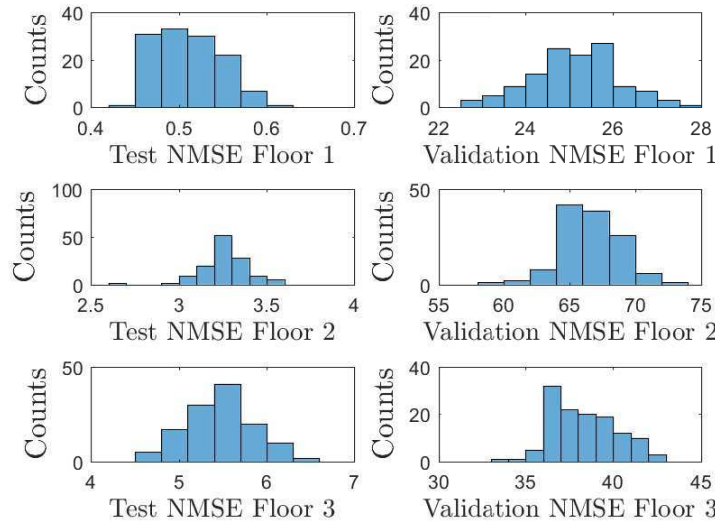


Fig. 13: NMSE for the MCMC acceleration predictions for each floor on the test (no 'bumper' contact)and validation ('bumper' contact) data sets

597 leading to ten lags being used as inputs.

598 Three GP models were generated (due to the single output nature of the GP). Each GP has a zero mean and Matérn
 599 3/2 covariance function prior. The covariance function is formulated using the automatic relevance detection form, where
 600 a length scale is placed for each input, allowing lag selection to be performed within the covariance function. For more on
 601 Gaussian Process regression the reader is referred to [93].

602 Each GP model was trained on sample points 200 to 400 of the training data set, such that the transients were removed
 603 and that the training data set did not being prohibitively large. Once trained the data-augmented model was used to predict
 604 on the test (where the 'bumper' mechanism is not in contact) and validation data (where 'bumper' mechanism is in contact)
 605 sets. The prediction for the test and validation cases are displayed in Figs. 14 and 15 respectively.

606 The NMSEs for the training, testing and validation sets were: $\{0.901, 0.386, 0.163\}$, $\{3.672, 2.426, 1.107\}$, $\{30.084, 39.837, 21.054\}$.
 607 This demonstrates that the data augmented model improved predictions for floors two and three (over both the MCMC and
 608 SADE prediction). However, the NMSE for floor one are larger than those from the previous analyses. This is likely due to
 609 the lack of dynamic information contained within the floor one location due to the positioning of the force.

610 Nonetheless, the data-augmented model provides additional benefits. The variance in the model reflects whether the GP
 611 has seen the combination of lagged inputs before. It would be expected that when the harsh nonlinearity was present the

612 variance (or standard deviation) of the model would increase, indicating that the model is predicting in an unseen region.
 613 This is confirmed by Figs. 14 and 15. In the test scenario the standard deviations are small and relatively stationary for each
 614 floor. Yet, in the validation data set the standard deviation for the first and second floor predictions increases at the point
 615 in the data where contact occurred. This is a useful property for a digital twin as it informs about the presence of epistemic
 616 uncertainty.

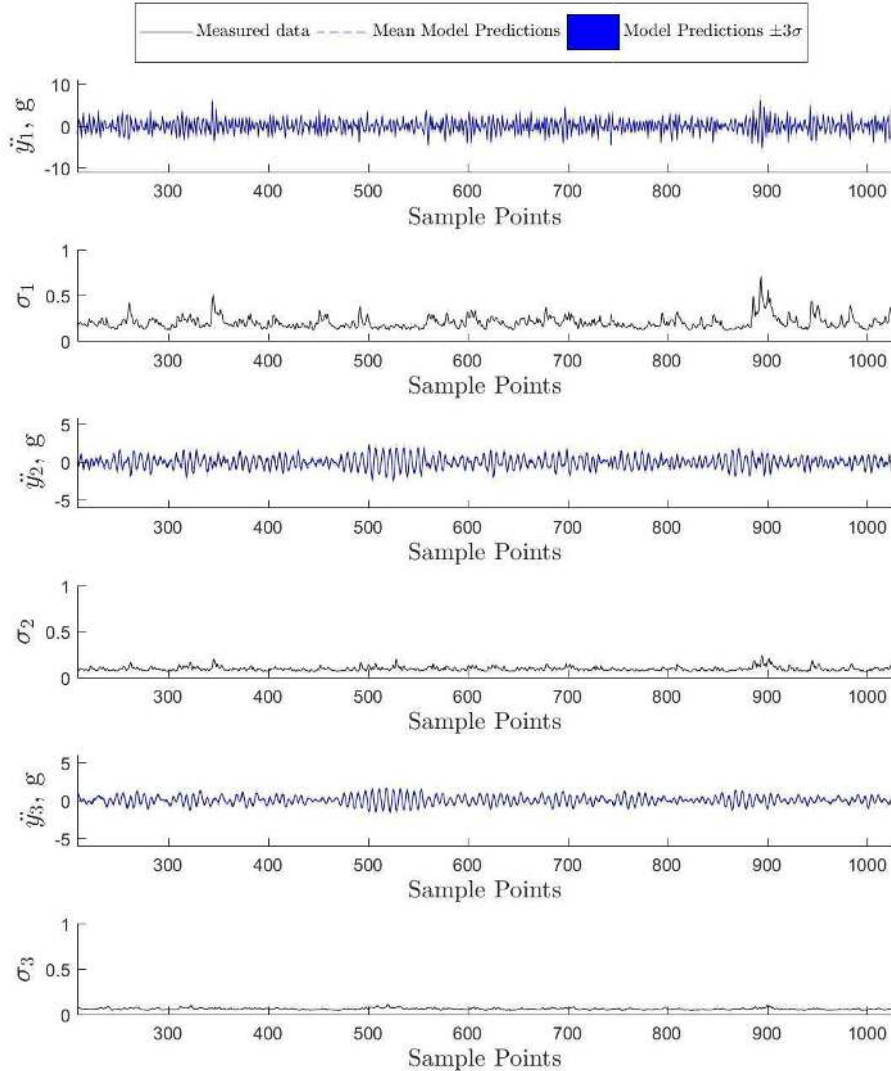


Fig. 14: Data augmented model predictions on testing data (no ‘bumper’ contact) and predictive standard deviations

617 The data augmented model can be used in an online manner to indicate when model improvements should be made.
 618 In regions of high variance the workflow could choose to re-perform the calibration step, or is could decide to improve the
 619 model form. For this example this could lead to a bilinear stiffness model being introduced in order to capture the contact
 620 behaviour. This would be a more optimal ‘white-box’ model and would help improve predictions in the validation data set.
 621 Unfortunately, the introduction of a nonlinear model would introduce new challenges in validation. For example, neither
 622 NMSE or model properties would be good validation metrics as both would fail to inform whether the bifurcation point had
 623 been correctly inferred. More sophisticated would be required, otherwise the model may perform extremely badly around
 624 the bifurcation point.

625 In addition, if the nonlinearity in the data set were a breathing crack the data-augmented model would have a method in
 626 triggering a warning that the structure was damaged. By performing outlier analysis on the predictive standard deviation, for

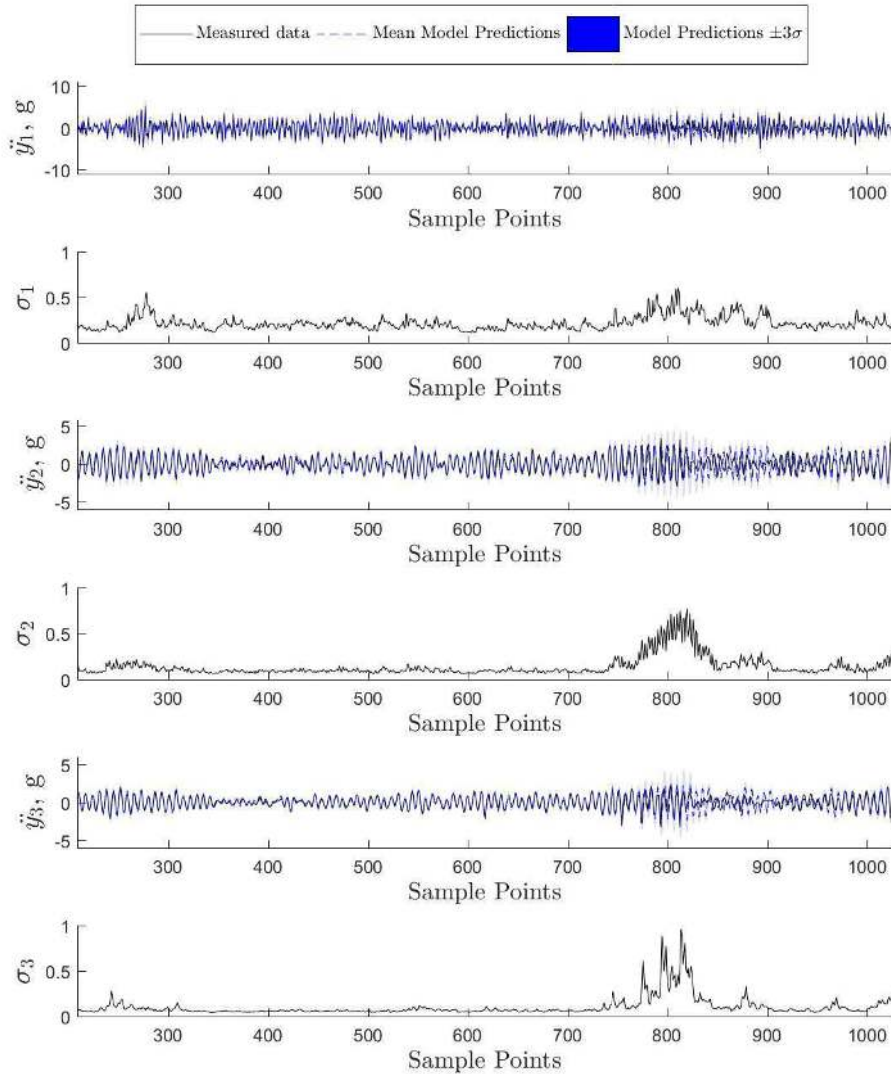


Fig. 15: Data augmented model predictions on validation data ('bumper' contact) and predictive standard deviations

627 example using a Mahalanobis distance, structural health monitoring decision can be made from the digital twin.

628 In conclusion, this case studies demonstrates that by moving up the levels of a digital twin more information and
 629 improved decision making can be made. This will allow, not only better more realistic predictions, but improved decision
 630 capabilities as well.

631 7 Open research problems and technological challenges

632 7.1 Workflow, coordination and time evolution

633 At its core, a digital twin needs to be able to coordinate multiple tasks simultaneously. It must respond to requests from
 634 the user, in addition to continuously coordinating background tasks such as gathering and processing data from the physical
 635 twin, and updating models and databases. For many applications, all other tasks except for this central coordination and
 636 management of workflows will be existing technology.

637 From a research perspective, there has been much recent work on workflows and related areas such as business process
 638 models [65–67,70]. In the context of a digital twin, these are potentially most useful during the asset management phase. The
 639 types of open questions still to be answered include how workflows can be most efficiently implemented, ensuring that they
 640 are sound and robust [71,73,94]. For this purpose, formalisations of network theory appear to be the most relevant tool [95].
 641 Furthermore, there is the question of how the workflow might *navigate* through the different elements of the digital twin,

642 and for this purpose using the idea of a *knowledge graph* (possibly built from an initial ontology) appears to be one practical
643 solution [96–98]. There is also the interesting question of how workflows can be adapted during the time evolution of the
644 digital twin [72]. A key element of the digital twin functionality is decision support, and as well as other factors such as
645 V&V, this also relates to the workflow processes [69, 99, 100].

646 Supporting all workflow processes in the digital twin will be a series of databases; these could be standalone, or online.
647 How these databases interface with the digital twin (beyond just providing raw data) is an area of research interest. In
648 particular, the use of knowledge graphs and ontologies [68], and ontology-driven databases appears promising. There is also
649 the interesting question of how much the digital twin makes use of processes such as data mining [101] via tools such as the
650 semantic web [102]; this also relates to the digital twin as part of the Internet of Things. [34].

651 7.2 Joints and joining

652 In Section 1, mechanical joints were highlighted as a technical example of a model ingredient for a digital twin. Along-
653 side that example, the issue of silos existing in organisations based on natural subdivisions in a particular application was
654 also discussed. Within the context of a digital twin there are some parallels between these two examples. The commonality
655 comes from the fact that subdivisions of many engineering systems are very natural – after all, complex systems are typically
656 made from multiple components and smaller sub-assemblages, which can naturally be modelled as simpler systems than the
657 full system. However, the sub-assemblages can often be considerably complex in their own right, and so once subdivided,
658 its not surprising that more focus goes into modelling the sub-assemblage rather than how it interacts with or is joined to
659 the rest of the system. Often, the associated models are incompatible in terms of jointing, and a bespoke interface model is
660 needed to try and connect the software models.

661 For the mechanical joints problem, there is already considerable research work that has been carried out — see for
662 example [103–105] and references therein. Dealing with the multi-scale and multi-physics nature of this problem is at the
663 heart of the newly developed research. The possibility of making predictions based on only a partly assembled structure, is
664 an interesting area of future research, and relates to the verification and validation models discussed in Section 2.2.

665 In terms of the working in silos and interfacing software based models, both problems can be thought of as problems
666 relating to *connectivity*. Many practitioners and researchers have already recognised these issues, and attempted to address
667 them using more integrated procedures, as described for example in [48] as part of the product lifecycle management (PLM)
668 ethos. Ensuring that this factor is taken into account when developing a digital twin is largely a question of implementing
669 current best practice [106, 107], but there are always potential improvements that can be made, and this will form an ongoing
670 research topic.

671 7.3 Uncertainty management and the quantification of trust

672 It has been highlighted throughout this paper that an important issue is how to deal with uncertainty within the digital
673 twin. In Section 6 a detailed example was presented that included a data-augmented modelling approach to managing the
674 uncertainties. This is just one approach amongst many available, as briefly discussed in Section 6.3. However, it should
675 be acknowledged that the example presented is relatively simple compared to most real engineering structures. For more
676 complex structures, an ongoing area of research will be determining how exactly uncertainties are propagated through a
677 digital twin in order to assess the level of confidence that can be given to the subsequent predictions.

678 In addition, enabling trust in digital twin predictions is essential to support engineering decision makers, see for example
679 [108]. To achieve this objective, the trust that can be ascribed to predictions from the digital twin must be quantified, and
680 for this it is essential to integrate techniques from uncertainty quantification and propagation [109–112]. This quantification
681 has to be an integral part of the digital twin, (an early example is given by [42]). An area of future work to facilitate this will
682 be to develop a risk based framework for the digital twin. Better assessment of potential risks, will help quantify trust, and
683 support decisions.

684 8 Conclusions

685 In this paper the application of the digital twin concept to engineering dynamics problems has been considered in
686 detail, with a particular emphasis on modelling and simulation. A description of the current state-of-the-art in this research
687 area, including a detailed literature review was presented. This included the background and history of the digital twin,
688 with particular emphasis on the topics of structural life prediction and verification & validation. Following this, a method
689 for synthesising a digital twin was presented, considering both design and asset management phases of the physical twin.
690 Five levels of sophistication for a digital twin were defined, along with essential elements and required processes using the
691 example of a simulation digital twin for a wind turbine. Methods for incorporating a digital twin into a product design
692 phase were discussed in the context of verification and validation procedures that can be carried out in parallel with design
693 and manufacture. To illustrate the detail of how several required processes could be implemented, an example case study
694 of a three-storey small-scale building was presented. This included a detailed description of data-augmented modelling to

695 manage uncertainty present in the structure. Finally, three of the open research problems and technological challenges were
696 outlined.

697 There are several key aspects that characterise the digital twins considered in this paper:

- 698 1 A structured coordination of all the required processes via a bespoke workflow which provides both the interface with
699 the user, and also the simultaneous integration of all other required processes (either bespoke or via software).
- 700 2 Quantification, management and ultimately reduction of model form (and other) uncertainties by use of measured data
701 from the physical twin.
- 702 3 Time-evolution of the digital twin in order to reflect the ageing of the physical twin, including the use of measured data
703 to update and evolve the physics-based models in the digital twin.
- 704 4 Robust methods for dealing with joints between parts of the physical twin.

705 In addition to this, methods from natural computing, (such as machine learning) are already being used for the data-based
706 techniques in this area, and the development of learning capabilities more generally is another area for future development.
707 This paper has focused on the largely philosophical aspects of the topic. It's clear from the current interest in this topic that
708 digital twin is set to have a disruptive influence on engineering applications. In a companion paper, as part of this special
709 issue, a mathematical framework for digital twin applications is developed, and together the authors believe this represents a
710 firm framework for developing digital twin applications in the area of engineering dynamics.

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