

# kPWORKBENCH: A Software Suit for Membrane Systems

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## Abstract

*Membrane computing* is a new natural computing paradigm inspired by the functioning and structure of biological cells, and has been successfully applied to many different areas, from biology to engineering. In this paper, we present kPWORKBENCH, a software framework developed to support membrane computing and its applications. kPWORKBENCH offers unique features, including *modelling*, *simulation*, *agent-based high performance simulation* and *verification*, which allow modelling and computational analysis of membrane systems. The kPWORKBENCH formal verification component provides the opportunity to analyse the behaviour of a model and validate that important system requirements are met and certain behaviours are observed. The platform also features a property language based on natural language statements to facilitate property specification.

*Keywords:* membrane computing, modelling, simulation, agent-based simulation, high performance simulation, verification, synthetic biology

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## 1. Motivation and significance

In order to go beyond the boundaries of conventional computer science and to be able to address more challenging problems, researchers have extensively worked on introducing new computational models and algorithms inspired from biological, physical, and chemical systems. *Membrane computing* [1] is a branch of nature inspired computing, aiming to develop computational models, methods and techniques by studying biological systems.

8       The central modelling formalisms within this paradigm are called *mem-*  
9 *brane systems* or *P systems*, and are inspired by the functioning and struc-  
10 ture of biological cells. P systems provide a mapping between biological cells  
11 and membranes, which are the computational units of the formalism. Several  
12 variants of P systems have been introduced and studied to model and analyse  
13 different problems, e.g., systems and synthetic biology [2, 3], synchronisation  
14 of distributed systems [4], optimisations and graphics [5].

15       In the last twenty years apart from introducing and studying many vari-  
16 ants of membrane systems [6], a number of tools have been built in order  
17 to support both theoretical investigations, but also practical applications –  
18 a thorough overview of most of the tools in this area is presented in [7].  
19 Amongst the most important tools produced so far are those widely used in  
20 applications. One such tool is P-Lingua [8, 9] covering a broad range of mem-  
21 brane systems and using an integrated platform, called MeCoSim [10]; the  
22 tool is specifically utilised in modelling and simulation of various biological  
23 systems. Another tool used to model biological systems is Meta PLab [11]  
24 which deals with a special class of P systems, called MP systems [12]. Also,  
25 numerical P systems, used in modelling and simulation of robot controllers  
26 benefit from a tool called SNUPS [13]; and hybrid P systems are supported  
27 by a simulator, called UPSimulator [14].

28       While the introduction of new variants allowed modelling different sets of  
29 problems, the ad-hoc addition of new features has caused an abundance of P  
30 system variants, with a lack of a coherent integrating view and well-defined  
31 framework that would allow us to analyse, verify and validate the systems  
32 behaviour.

33       To address these issues, we have introduced *kernel P systems (kP sys-*  
34 *tems)* [15, 16] to create more general membrane computing models, inte-  
35 grating the most used concepts from P systems. The expressive power and  
36 efficiency of the newly introduced kP systems have been illustrated by a num-  
37 ber of representative case studies [15, 17, 18, 19]. In this respect, we have  
38 also introduced a modelling language, called *kP-Lingua*, allowing to write  
39 kP system models. The theoretical aspects of the methods and techniques  
40 developed for kP systems have been discussed in [20, 21, 22, 23].

41       To provide a tool support for this framework, we have developed the  
42 kPWORKBENCH platform (available and downloadable from its website [24]),  
43 which permits modelling and computational analysis of membrane systems  
44 through its unique features, *modelling, simulation, agent-based high perfor-*  
45 *mance simulation* and *verification*. To assist users in verification process,  
46 which is a very cumbersome process for non-experts, the platform also fea-  
47 tures a user friendly property language based on *natural language* statements,  
48 which makes the property specification a much easier task. These unique

49 features make kPWORKBENCH the only available tool supporting the non-  
 50 probabilistic modelling and analysis of membrane systems using various com-  
 51 putational approaches. The usability and novelty of our approach have been  
 52 illustrated by some case studies from systems and synthetic biology [17, 18]  
 53 to some engineering problems [25, 19].

## 54 2. Software description

55 This paper presents the first stable software release of kPWORKBENCH,  
 56 a software platform that integrates a set of tools and methods, allowing one  
 57 to *model* membrane systems and to analyse them through *simulation*, *agent-*  
 58 *based high-performance simulation* and *verification*.

### 59 2.1. Software Architecture

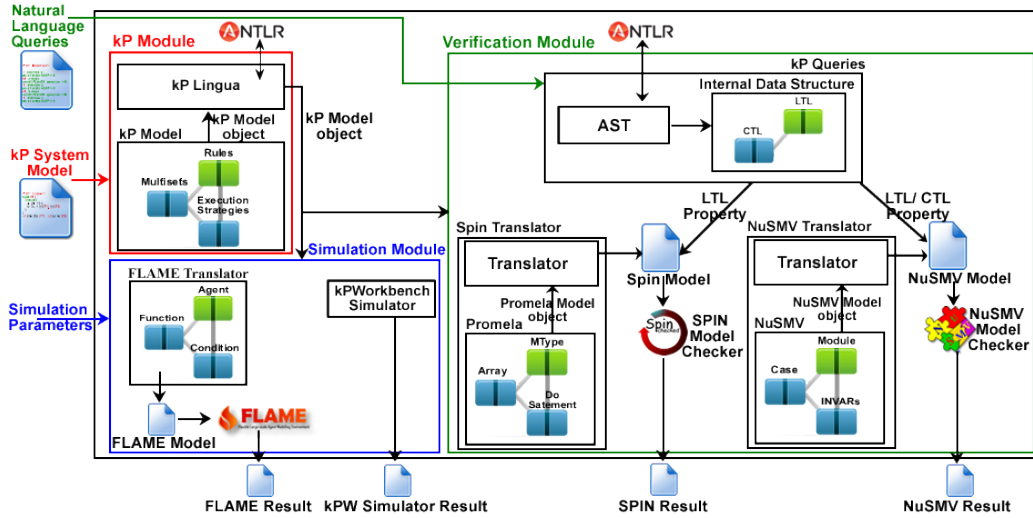


Figure 1: The overview architecture of kPWORKBENCH framework.

60 Figure 1 depicts an overview of the kPWORKBENCH system architecture,  
 61 which consists of three modules:

- 62 **1. The kernel P (kP) module** takes a kP system model specified in  
 63 kP-Lingua, which can be created or edited using a dedicated model editor,  
 64 as input. The grammar of the kP-Lingua language is written in ANTLR  
 65 (ANother Tool for Language Recognition) [26], automatically generating the  
 66 necessary syntactical and semantic analysers. The *kP Model* module accom-  
 67 modates the corresponding data structures of the input model, comprising

68 compartment types, execution strategies, rules, multiset of objects and con-  
69 nections between compartments. The kP–Lingua module instantiates a kP  
70 Model object and maps the AST (abstract syntax tree) generated by ANTLR  
71 to that object. This object is used as Data Transfer Object (DTO) between  
72 different modules of the framework. This separation helps developers easily  
73 adding new components to the framework.

74 **2. The *Simulation* module** consists of two components, kPWORKBENCH  
75 simulator and FLAME agent-based simulator [27]. Both require the kP  
76 Model object and simulator parameters, e.g. number of steps, as input.  
77 The kPWORKBENCH Simulator component is a custom simulator, which  
78 processes the multisets of objects of the input model with respect to its  
79 execution strategies and rules. The FLAME Translator transforms the kP  
80 Model object into a FLAME Model object that aggregates agent, function,  
81 input, condition and output classes. It assigns each compartment to an agent,  
82 and the rules and the multiset of objects are stored as agent data. It creates a  
83 specific function for each type of execution strategy. In addition, it creates C  
84 functions that represent the system behaviour (they are executed by FLAME  
85 when the agent makes a transition from one state to another). The FLAME  
86 Translator uses the ANTLR template group feature to produce the FLAME  
87 simulator specifications from the FLAME Model object.

88 **3. The *Verification* module** contains three components: the SPIN [39]  
89 and NUSMV [40] translators and the *kP Queries* module:

90 The SPIN Translator has two main components: *Translator* and *Promela*  
91 (SPIN’s specification language). The Translator maps the kP Model object  
92 to a *Promela* object using the following procedure [20]:

- 93 (i) A compartment type is translated into a data type definition with the  
94 multiset of objects and links to other compartments, and also with  
95 temporary storage variables that provide the parallelism of P systems.
- 96 (ii) Multiset of objects is assigned to an integer array where an index de-  
97 notes the object and its value represents the multiplicity of the object.
- 98 (iii) The set of rules are organised according to the execution strategies  
99 mapped by a *Proctype* definition – a Promela process.
- 100 (iv) Maximal parallelism and arbitrary execution strategies are mapped to  
101 the *Do* statement, and choice execution strategy is mapped to *If* state-  
102 ment.

103 After the mapping process, the *Translator* component translates the  
104 Promela object to the corresponding Promela model, used by the SPIN model  
105 checker. More details about the translation from kP System model to the  
106 SPIN model checker specification can be found in [20].

107 Similarly, the NuSMV Translator translates the kP Model object to the  
 108 corresponding NuSMV representation (NuSMV's specification language).  
 109 The translator has two main components: *Translator* and NuSMV. The  
 110 NuSMV component consists of subcomponents representing the NuSMV  
 111 language objects. The *Translator* maps the kP Model object to the NuSMV  
 112 object as follows:

- 113 (i) Each compartment is translated into a module.
- 114 (ii) The content of compartments is translated into variables.
- 115 (iii) The initial multisets of the compartment are assigned into module pa-  
 116 rameters.
- 117 (iv) Rules and guards are translated into the case statements.
- 118 (v) The behaviour of execution strategies and the parallelism of P systems  
 119 are achieved by introducing custom variables.

120 After the mapping process, the Translator component generates the NuSMV  
 121 model from the NuSMV object.

122 The *kP-Queries* module receives a property, a natural language based  
 123 statement, as input. The user can build properties from the property lan-  
 124 guage editor. The editor interacts with the kP-Lingua model, and permits  
 125 accessing the native model elements, which simplifies the property building  
 126 process. The kP-Queries' domain language has its own grammar, which is in-  
 127 dependent from and much simpler than the target model checking languages.  
 128 The DSL (domain specific language) of the property language is written in  
 129 ANTLR, receiving the EBNF grammar as input and generates the corre-  
 130 sponding syntactic and semantic analysers as well as the corresponding AST.  
 131 We use the *Visitor design pattern* approach, which enables the kP-Queries  
 132 module to translate every node of the internal presentation of property into  
 133 the target model checker's corresponding property specification language.

## 134 2.2. Software Functionalities

### 135 *Modelling.*

136 kPWORKBENCH accepts kP system models specified in an intuitive mod-  
 137 elling language, *kP-Lingua*. kP systems accumulate the most important as-  
 138 pects of various P system variants, so kP-Lingua provides a generic language  
 139 to model various membrane systems. kPWORKBENCH features a graphical  
 140 model editor, permitting to create new model files and editing existing files.

### 141 *Simulation.*

142 kPWORKBENCH offers two different approaches to simulate kP systems.  
 143 In both approaches, a kP-Lingua model is provided as an input, and the

144 execution traces of the model are returned as an output. These traces permit  
 145 exploring the dynamics of the system and observing how the system evolves  
 146 over time.

147 In the first approach, we have developed a custom simulation tool [22],  
 148 which recreates the system dynamics as a set of simulation runs in a *sequential*  
 149 *way*. The tool translates a kP-Lingua specification into an internal data  
 150 structure, which permits representing compartments, containing multisets of  
 151 objects and rules, and their connections with other compartments.

152 In the second approach, we have integrated the FLAME simulator [28, 27],  
 153 a general purpose large scale agent based simulation environment. FLAME  
 154 is based on the X-machine formalism [29], a type of extended finite state  
 155 machine whose transitions are labelled by processing functions that operate  
 156 on a (possibly infinite) set called memory, that models the system data.

157 In order to simulate kernel P system models in a *parallel way* using  
 158 the FLAME framework, an automated model translation has been imple-  
 159 mented for converting the kP-Lingua specification into communicating X-  
 160 machines [29]. One of the main advantages of this approach is the high  
 161 scalability degree and efficiency for simulating large scale models.

## 162 *Verification.*

163 Verification, in particular model checking, has been widely applied to the  
 164 analysis of various systems [30, 31, 32, 33, 34]. Verification checks if system in  
 165 question meets user requirements, expressed in a formal logic [35, 36, 37, 38],  
 166 by exhaustively analysing all possible execution paths verification.

167 Utilising a comprehensive, integrated and automated verification approach  
 168 is a very challenging task in the context of membrane computing. For exam-  
 169 ple, it is very difficult to transform some complex features, e.g. membrane  
 170 division, dissolution and link creation/destruction, into suitable abstractions  
 171 in verification tools.

172 We have successfully addressed these issues, and developed a verification  
 173 environment for kPWORKBENCH, integrating some state of the art model  
 174 checking tools, e.g. SPIN [39] and NUSMV [40]. The translations from a  
 175 kP-Lingua representation to the corresponding SPIN and NUSMV inputs  
 176 (i.e. PROMELA and SMV, respectively) are automatically performed.

177 In order to facilitate the property specification task (a very difficult  
 178 process for non-experts who are not familiar with verification languages)  
 179 kPWORKBENCH features a user friendly property language, *kP-Queries*,  
 180 based on *natural language* statements. The language also provides a list of  
 181 property patterns (templates), generated from most commonly used queries.  
 182 The property language permits specifying the target logic (i.e. LTL and  
 183 CTL) for different properties without placing a requirement on a specific

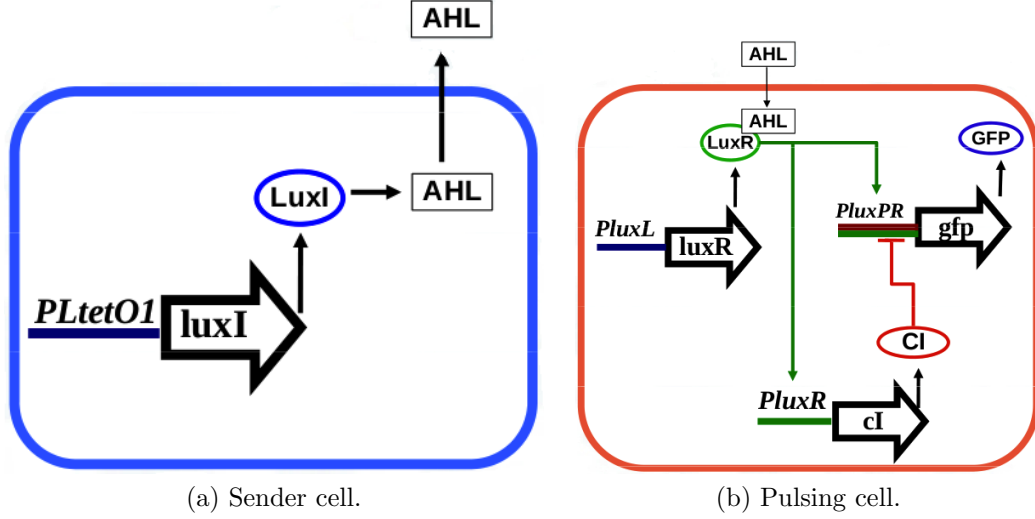


Figure 2: Two cell types of the pulse generator system.

184 model checker. In this way, we can use the same set of properties in various  
 185 verification experiments.

### 186 3. Illustrative Examples

187 In this section, we show the usability of kPWORKBENCH on a synthetic  
 188 biology case study [41, 18]. The *pulse generator* [42] is a synthetic biology sys-  
 189 tem, composed of two types of bacterial strains: *sender* and *pulsing* cells (see  
 190 Figure 2). The sender cells produce a signal (AHL) and propagates it through  
 191 the pulsing cells, which express the green fluorescent protein (GFP) upon  
 192 sensing the signal. The excess of the signalling molecules are propagated to  
 193 the neighbouring cells. Sender cells synthesise the signalling molecule AHL  
 194 through the enzyme LuxI, expressed under the constitutive expression of the  
 195 promoter PLtetO1. Pulsing cells express GFP under the regulation of the  
 196 PluxPR promoter, activated by the LuxR\_AHL<sub>2</sub> complex. The LuxR protein  
 197 is expressed under the control of the PluxL promoter. The GFP production is  
 198 repressed by the transcription factor CI, codified under the regulation of the  
 199 promoter PluxR that is activated upon binding of the transcription factor  
 200 LuxR\_AHL<sub>2</sub>.

201 For this case study, we have designed a membrane system, which is a  
 202 lattice comprising 1 sender cell and 10 pulsing cells in a sequential order.  
 203 Through simulation and verification experiments, we have observed the prop-  
 204 agation of the signalling molecules from the sender cells to the pulsing cells.

Table 1: Simulation results.

Step Interval	sender <sub>1</sub>	pulsing <sub>10</sub>	
	AHL	AHL	GFP
0 – 10,000	Exist	None	None
10,001 – 20,000	Exist	Exist	None
20,001 – 30,000	Exist	Exist	None
...	...	...	...
80,001 – 137,178	Exist	Exist	None
137,179 – 150,000	Exist	None	Exist

205 The system is modelled in kernel P systems using the kP–Lingua language.  
 206 The actual kP–Lingua model can be accessed at [43].

### 207 *Simulation*

208 The simulation components of kPWORKBENCH are used to explore the  
 209 temporal evolution of the system and to infer various information from the  
 210 simulation results. By analysing the execution steps, we can explore the  
 211 dynamic behaviour of the system in question.

212 Table 1 presents the production and availability of the signalling molecules  
 213 in the sender cell (i.e. **sender<sub>1</sub>**) and the transmission of the signalling  
 214 molecules and the production of the green florescent protein in the furthest  
 215 pulsing cell (i.e. **pulsing<sub>10</sub>**). The simulation results show that the signalling  
 216 molecule can be produced and transmitted by the sender cell on average  
 217 within 10,000 steps. The furthest pulsing cell will eventually receive these  
 218 signalling molecules (between 10,001 and 20,000 steps), and can use the signal  
 219 for the production of **GFP** in later steps (after 137,179 steps), which confirms  
 220 the propagation behaviour.

221 The simulation presented in Table 1 is a sequential process, which is not  
 222 very efficient for large systems, e.g. biological systems. The FLAME sim-  
 223 ulator provides a much faster and efficient alternative for large systems as  
 224 it uses parallel algorithms, run in high performance environments. Figure 3  
 225 compares the performance of the kPWORKBENCH native simulator (sequen-  
 226 tial simulation) and FLAME simulator (parallel simulation). As the number  
 227 of cells increases, FLAME runs significantly faster than the kPWORKBENCH  
 228 simulator.

### 229 *Verification*

230 The verification component allows us to check if a model satisfies the  
 231 system requirements. In order to observe the propagation behaviour of the



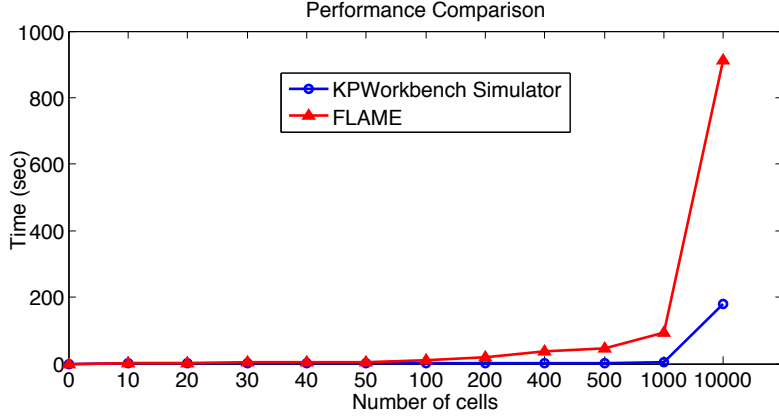


Figure 3: The comparative simulation results for kPWORKBENCH and FLAME.

Table 2: Verified properties.

#	Description	kP-Queries	Result
1	<b>AHL</b> is eventually propagated to <b>pulsing<sub>10</sub></b>	ctl: eventually puls10.signalAHL > 0	T
2	<b>GFP</b> is eventually produced in <b>pulsing<sub>10</sub></b>	ctl: eventually puls10.proteinGFP > 0	T
3	<b>AHL</b> in <b>pulsing<sub>1</sub></b> is followed by <b>AHL</b> in <b>pulsing<sub>10</sub></b>	ctl: puls1.signalAHL > 0 followed-by puls10.signalAHL > 0	T
4	<b>AHL</b> in <b>sender<sub>1</sub></b> is followed by <b>GFP</b> in <b>pulsing<sub>10</sub></b>	ctl: send1.signalAHL > 0 followed-by puls10.proteinGFP > 0	T
5	<b>GFP</b> in <b>pulsing<sub>10</sub></b> is preceded by <b>AHL</b> in <b>pulsing<sub>9</sub></b>	ctl: puls10.proteinGFP > 0 preceded-by puls9.signalAHL > 0	T

232 pulse generator system, we have written some properties in kP-Queries and  
 233 verified them on the kP-Lingua model.

234 Table 2 shows the verification results. The first column shows the prop-  
 235 erty number; the second column describes the properties informally; the third  
 236 column shows the formal properties expressed in kP-Queries (which are then  
 237 automatically translated into CTL in NuSMV syntax); and the last column  
 238 presents the verification results. Property 1 and 2, respectively, verify that  
 239 **AHL** is eventually propagated to the furthest pulsing cell, which then pro-  
 240 duces **GFP** upon sensing the signalling molecules. Property 3 verifies that  
 241 **AHL** propagates through the lattice. Property 4 proves that the sender cell  
 242 starts the expression of **AHL**, which then triggers the production **GFP** in the  
 243 pulsing cells. Finally, Property 5 proves that **AHL** should be sensed in the  
 244 previous neighbouring cell before **GFP** is produced in the next cell.

## 245 4. Impact and conclusions

246 In this paper, we have discussed a nature inspired computing paradigm,  
247 membrane computing, and the kPWORKBENCH software platform developed  
248 to support it.

249 The need to build tools supporting the membrane computing research  
250 has been identified quite early and presented in [6]. The current state of the  
251 art development of membrane computing tools [7] refers to a broad spectrum  
252 of topics covered. The vast majority of these tools concentrate on a specific  
253 variant or a set of variants of membrane systems. Compared with the rest  
254 of membrane computing tools, kernel P systems provide more general mem-  
255 brane computing models, integrating the most used concepts from P systems.  
256 This is an important aspect of the research within the membrane computing  
257 community, as outlined in a survey paper [44].

258 kPWORKBENCH integrates several state-of-the-art simulation and verifi-  
259 cation tools and methods. Featuring multiple simulators, using a native pro-  
260 cess and agent-based approaches relying on sequential and high performance  
261 execution, is very unique in this field. These features allow kPWORKBENCH  
262 to efficiently express problems studied with other classes of membrane sys-  
263 tems, consequently analyse them via simulation and verification and decide  
264 on the best solutions.

265 The formal verification feature, which does not exist in any other mem-  
266 brane computing tools, provides the opportunity to analyse the system be-  
267 haviour and check if certain properties about the system specification are  
268 verified, which cannot be done using the conventional simulation approach.  
269 Another unique feature is the user-friendly property specification process us-  
270 ing natural language statements, making the property specification very easy  
271 for non-experts. These features make kPWORKBENCH the only available in-  
272 tegrated toolset permitting non-deterministic analysis of membrane systems.

273 kPWORKBENCH has been used in computational modelling and analy-  
274 sis of various systems, providing insights into their behaviour. This helps  
275 formulating new research questions and addressing them within an efficient,  
276 robust and rigorous environment.

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396 **Current code version**

397 **Current executable software version**

<b>Nr.</b>	<b>Code metadata description</b>	<b>Please fill in this column</b>
C1	Current code version	v1.0
C2	Permanent link to code/repository used for this code version	<a href="https://git.io/JeRDD">https://git.io/JeRDD</a>
C3	Code Ocean compute capsule	<a href="https://bit.ly/33Arx0l">https://bit.ly/33Arx0l</a>
C4	Legal Code License	MIT License
C5	Code versioning system used	git
C6	Software code languages, tools, and services used	.Net Core, C#, Spin, Promela, NuSMV, FLAME, ANTLR
C7	Compilation requirements, operating environments & dependencies	<a href="https://git.io/JeRDD">https://git.io/JeRDD</a>
C8	If available Link to developer documentation/manual	
C9	Support email for questions	<a href="mailto:l.m.mierla@bradford.ac.uk">l.m.mierla@bradford.ac.uk</a>

Table 3: Code metadata (mandatory)

<b>Nr.</b>	<b>(Executable) software meta-data description</b>	<b>Please fill in this column</b>
S1	Current software version	kPWorkbench v1.0, kPWorkbench UI v1.0
S2	Permanent link to executables of this version	<a href="https://git.io/Je2Fa">https://git.io/Je2Fa</a>
S3	Legal Software License	MIT License
S4	Computing platforms/Operating Systems	kPWorkbench: Linux x64, OS X x64, Windows x64; kPWorkbench UI: Windows x64
S5	Installation requirements & dependencies	<a href="https://git.io/JeRDD">https://git.io/JeRDD</a>
S6	If available, link to user manual - if formally published include a reference to the publication in the reference list	<a href="https://git.io/JeRDD">https://git.io/JeRDD</a> , <a href="https://git.io/Je2Fr">https://git.io/Je2Fr</a>
S7	Support email for questions	<a href="mailto:l.m.mierla@bradford.ac.uk">l.m.mierla@bradford.ac.uk</a>

Table 4: Software metadata (optional)