



# Modeling complex systems in animal science: A pedagogical framework for new researchers

Luis Orlando Tedeschi<sup>1\*</sup> , Dan Tulpan<sup>2</sup> , Hector M. Menendez III<sup>3</sup> ,  
Ricardo Augusto Mendonça Vieira<sup>4</sup> 

<sup>1</sup> Texas A&M University, Department of Animal Science, College Station, TX, USA.

<sup>2</sup> University of Guelph, Department of Animal Biosciences, Guelph, ON, Canada.

<sup>3</sup> South Dakota State University, Department of Animal Science, Rapid City, SD, USA.

<sup>4</sup> Universidade Estadual do Norte Fluminense, Laboratório de Zootecnia, Campos dos Goytacazes, RJ, Brasil.

\*Corresponding author:  
[luis.tedeschi@tamu.edu](mailto:luis.tedeschi@tamu.edu)

Received: October 7, 2024

Accepted: February 4, 2025

**How to cite:** Tedeschi, L. O.; Tulpan, D.; Menendez III, H. M. and Vieira, R. A. M. 2025. Modeling complex systems in animal science: A pedagogical framework for new researchers. Revista Brasileira de Zootecnia 54:e20240170. <https://doi.org/10.37496/rbz5420240170>

## Editors:

Mateus Pies Gionbelli

Marcos Inácio Marcondes

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**ABSTRACT** - Mathematical modeling is a systematic process that involves identifying key variables and understanding how they interact. This review provides a comprehensive pedagogical framework for new researchers in animal science modeling, addressing the critical gap between general modeling theory and domain-specific applications. While modeling typically begins with conceptualization using visual aids such as causal loop diagrams, stock and flow diagrams, mind maps, and flowcharts to organize relationships among variables, there is a notable lack of resources that effectively bridge theoretical concepts with practical applications in animal science. This process allows scientists to build simplified representations of complex systems while providing structured guidance specifically tailored to biological systems. Modelers must balance simplicity and complexity to maintain functionality while reflecting real-world systems. Simple models, though limited, offer greater usability and interpretability, while complex models can become challenging to apply practically. After translation to mathematical form and computer code, models undergo rigorous parameterization with real-world data, evaluation against independent datasets, and sensitivity analyses. Models challenge our understanding, reveal knowledge gaps, and guide research. By embracing an iterative approach to model development—in which refinement and improvement are continuous—researchers can develop models that are not only accurate and predictive, but also practical and usable in addressing real-world challenges. This continuous development cycle, evaluation, and application ensures that models remain relevant and capable of evolving alongside scientific knowledge and technology advancements.

**Keywords:** agricultural system, animal nutrition, modeling

## 1. Introduction

Contrary to widespread belief, mathematical modeling (MM) and, more recently, computational modeling are fundamentally simple and accessible processes. At its core, modeling merely requires a systematic identification of critical variables and a clear understanding of how these variables relate to each other. This simplicity is often obscured by the perceived complexity of advanced models, leading many to view modeling as an intricate, specialized skill. In reality, the basic principles of modeling are straightforward: identify the essential elements of a system and map out how they interact. Systems thinking (ST) and design thinking (DT) are two logical thinking methodologies that follow structured approaches to problem-solving, grounded in reasoning and logic.

Prior to analyzing the relationship and differentiating between the two methodologies, it is essential to define what we mean by “system”—a set of interconnected components that function together as a whole, bounded by defined scope and purpose. In animal science, a system might range from a specific metabolic pathway to an entire farm operation. Buchanan (2019) identified four key aspects that must be addressed when working with systems: system boundaries and scope (what we include or exclude in our abstract representation of reality), the system parts that can be systematized, the overarching understanding of how system parts work together, and the purpose of the system. The first issue is perhaps the most important to clarify since we comprehend the surrounding world by observing phenomena and aim to explain them by conceptualizing systems. Nevertheless, their origins and constituent components might not be obvious and, therefore, hard to define and distinguish. Assuming the first one was clarified, the second issue resides in identifying the system components that require consideration. System components could be organic (people, animals) or inorganic (objects), material (physical environments) or immaterial (ideas, beliefs, practices), or perhaps of a different nature (e.g., grouped by levels of complexity, uncertainty, decision, or change); nevertheless, being aware of their existence influences our understanding of how to model such systems better. The third issue focuses on understanding how system components interact, interdepend, and work together to further our understanding of the system’s overall functionality. Notions such as structural hierarchies, openness, closeness, presence or absence of resilience to external and internal disturbances, and the ability to self-organize, adapt, and evolve need to be acquired before modeling the system. Last, we must distinguish between the system’s *raison-d’être* (e.g., how a metabolic pathway naturally operates to maintain homeostasis) and the modeler’s purpose in studying it (e.g., optimizing feed efficiency or reducing methane emissions). While the system operates independently of our interest in it, the modeler’s objectives influence which aspects of the system are considered most relevant for inclusion in the model, allowing us to focus specifically on the components essential to addressing the research questions at hand. Both perspectives are critical to achieving realistic modeling results. While ST has been widely applied in teaching and learning contexts (Zhang and Ahmed, 2020), DT shares its principles and has recently gained popularity, specifically in developing capstone courses (Donaldson and Smith, 2017). However, they apply logic differently based on their core principles.

In this review, we define model complexity in terms of three key dimensions: the number of variables and parameters involved, the nature of relationships between components (linear vs. non-linear interactions), and the structural hierarchy of the model (e.g., nested processes, feedback loops, and multi-scale interactions). Complex models typically feature numerous interacting variables, non-linear relationships, and hierarchical structures spanning multiple biological scales. For example, a complex model of ruminant nutrition might incorporate dozens of variables representing nutrient flows, multiple non-linear enzymatic reactions, and hierarchical processes ranging from molecular metabolism to whole-animal performance.

The field of animal science modeling faces unique challenges that distinguish it from other modeling domains. These challenges include, but are not limited to, the inherent variability of biological systems; the complexity of interactions among nutrition, genetics, and environment; and the practical constraints of data collection in livestock systems. While general modeling principles provide a foundation, their application in animal science requires specific considerations and adaptations. This review addresses the gap between theoretical modeling frameworks and their practical implementation in animal science, providing structured guidance for researchers new to the field. By systematically connecting fundamental modeling concepts with animal science applications, we present a comprehensive pedagogical framework that enables new researchers to develop effective, scientifically sound models, while avoiding common pitfalls specific to biological systems modeling.

This review has three specific objectives: to provide a structured pedagogical framework connecting general modeling principles with animal science applications, addressing the current gap between theory and practice; to guide new researchers through the systematic process of developing, evaluating, and implementing mathematical models specifically for biological systems in animal science; and to highlight the unique challenges and considerations in animal science modeling that distinguish it

from other modeling domains. By achieving these objectives, this review provides a comprehensive resource that bridges the gap between theoretical modeling concepts and their practical application in animal science research.

### 1.1. Balancing model complexity and usability

Balancing model complexity and usability is crucial because it ensures that models are both scientifically robust and practical for real-world applications. Mazzocchi (2008) proposes a balanced approach to modeling, advocating for integrating reductionist and holistic methodologies. He argues that while reductionism allows for the dissection of individual components of a system, a holistic view is necessary to understand how these components interact within the broader context. This perspective offers a more comprehensive understanding of complex systems and avoids the pitfalls of oversimplification. His viewpoint differs from Tedeschi's (2023b) viewpoint, who argued that reductionist models, especially in biological and agricultural sciences, are effective tools for organizing complex data and generating valuable predictions. While both approaches recognize the value of simplification, Mazzocchi's (2008) critique highlights the need to balance reductionism and system-level understanding, which may be particularly relevant as models evolve to incorporate broader ecological and environmental considerations. As models grow more complex to reflect the intricate nature of systems, Tedeschi (2023b) contends that fully grasping all the interrelationships within the model becomes increasingly challenging, if not humanly impossible. A plethora of research also supports this idea focused on formal methods for software development of complex systems (Kneuper, 1997). This complexity not only complicates the interpretation of the model, but also renders the processes of parameterization, verification, validation, and evaluation far more difficult and time-consuming. In computational modeling, validation confirms that the code accurately reflects the intended equations and concepts, while evaluation tests the ability of the model to predict or explain observed outcomes based on the given inputs (Tedeschi, 2006). As a result, the practical usability of the model may be hindered, potentially making it less accessible to scientists and practitioners. While complexity is often necessary to capture the full scope of a system, it must be balanced with a consideration of usability, computational efficiency, and feasibility to ensure the model remains functional, provides timely results, and is not overly burdensome in real-world applications.

### 1.2. The modeling process and conceptualization

Embarking on developing a mathematical model is akin to setting out on an intellectual journey, in which each step forward may lead to new insights or challenges that prompt us to revisit our earlier assumptions. This process begins with curiosity or a pressing need to understand a complex system or phenomenon (Tedeschi, 2023b). The modeling process starts with clearly defining the problem at hand (Buchanan, 2019). We ask ourselves: What are we trying to understand or predict? What are the key elements at play? This initial phase of problem identification and formulation sets the stage for everything that follows. At this point, the modeler begins to sketch out the landscape of the model-to-be, identifying the key variables and parameters that will populate our mathematical terrain.

As we delve deeper, we enter the realm of conceptualization. This is where we begin to map out the relationships between our variables, much like an explorer charting the connections and pathways layout between different landmarks. We make decisions about what to include in our model and what to leave out, knowing that these choices will shape our entire journey. The process begins with identifying the most crucial variables or objects within the system being studied. These are then systematically arranged, often on a simple piece of paper, and connected with lines and arrows to indicate their relationships. This basic sketch forms the foundation of more complex models. The most commonly used schematics for this purpose are causal loop diagrams (CLD) and flowcharts. While these visual representations do not allow for numerical simulations on their own, as they lack specific values or mathematical formulas, they serve as invaluable tools for conceptualizing and communicating the underlying structure of a model.

The subjective nature of CLD, reflecting the modeler's state of mind, implies that multiple interpretations can exist for modeling the same behavior. This subjectivity has led to some debate within the scientific community regarding the extent to which models can accurately represent natural or real systems and their simulation or predictive capabilities. It is crucial to understand that the primary objective of a CLD (and a mathematical model based on it) is to document the modeler's conceptualization at a specific point in time rather than to represent an absolute reality. The development of both CLD and, ultimately, models is an iterative process that involves meticulous selection and connection of variables perceived as significant. Consequently, several iterations may occur before a "final" version is established, and different models may be created to represent the same problem or behavior mathematically. Swannack et al. (2025) emphasized a similar iterative approach in conceptual modeling, particularly for novice modelers transitioning from ecological systems to computational tools. Their work highlighted the importance of refining initial conceptual diagrams to focus on critical system components, thereby facilitating smoother transitions into the coding phase. This approach aligns with the structured use of CLD and other visual aids discussed in this review paper.

Mathematical models are, in essence, tools that enable scientists to document their understanding of a system coherently and visually (if graphical aids are used). When combined with mathematical formulations, these models can reveal patterns and trends generated by the system being studied. However, asking which model is "better" for a particular purpose without considering the context is the wrong question and is often misleading. Each model is built on different assumptions and perceptions intrinsic to its development and limited by the modellers' vision, knowledge, skills, and perception of reality and user needs. As a result, models may be biased or tailored for specific situations, potentially limiting their applicability to other scenarios beyond the one they were originally intended or envisioned for.

The true value of modeling—whether mathematical, computational, or conceptual—lies in its ability to challenge the perceived reality of both the modeler and the end-user. It compels them to confront discrepancies between their beliefs or limited understanding of reality and the model's predictions, prompting either a reevaluation of their understanding or a revision of the model itself. This process facilitates a deeper understanding of how variables interconnect within a particular problem. It is through this iterative, thought-provoking process of questioning our knowledge, examining relationships, identifying shortcomings, and recognizing knowledge gaps that modeling achieves its primary goal. This approach not only enhances our understanding of the limitations in our current knowledge but also guides the development of methodologies and experimental designs to address these gaps. By targeting our efforts, manpower, and financial resources more effectively, we can significantly advance scientific knowledge in fields such as animal nutrition.

## 2. Systems thinking vs. design thinking

Systems thinking is an analytical approach that views a problem or situation as part of an interconnected system. It is believed that Ludwig von Bertalanffy laid the groundwork for ST through his development of the "General Systems Theory" in the 1930s (Von Bertalanffy, 1968). However, Jay Forrester further advanced the field in the 1950s by focusing on understanding the behavior of complex systems over time, particularly in the context of industrial and organizational dynamics. He introduced the concept of feedback loops and emphasized the importance of considering the long-term impacts of decisions within a system (Forrester, 1961). The fundamental principles of ST are a holistic view to look at the whole system rather than isolated parts; interconnectedness for recognizing how different elements within the system influence one another; feedback loops for understanding how outputs of a system can influence its inputs in continuous cycles; and emergent behavior for acknowledging that the behavior of the system is often more complex than the sum of its parts. Systems thinking focuses on understanding how different parts of a system (i.e., things, objects, variables) interact and influence one another to generate outcomes. The key concept is that the behavior of a system's emerges from the interactions of its components, meaning that to solve problems effectively, the modeler must consider the system as a whole rather than just individual elements, while being mindful of the practical limitations

this holistic approach imposes on model usability and interpretability. Mazzocchi (2008) argued that holistic approaches in scientific reasoning, such as those found in ST, are crucial for addressing complexity in modern scientific problems. His work emphasizes that reductionist methods often fail to capture the emergent properties of systems, reinforcing the need for integrative approaches like ST, though this perspective overlooks the practical challenges of implementing highly complex models that Tedeschi (2023b) rightfully identified.

On the other hand, DT is a user-centered, problem-solving approach that focuses on innovation and creative solutions. Herbert A. Simon is often credited with introducing the concept of DT in 1969 (Simon, 1996), in which he described design as a way of thinking that involves devising courses of action aimed at changing existing situations into preferred ones. Design thinking emphasizes empathy with users, defining the problem from their perspective, brainstorming ideas, prototyping, and iteratively testing those ideas. It is often used to address complex problems by framing them in a human-centered way and applying a creative, experimental process to come up with new ideas. The fundamental principles of DT are empathy for understanding the needs and challenges of users; ideation for generating a wide range of potential solutions; prototyping for building tangible representations of ideas to test and iterate; and iterative processes for repeatedly refining and improving ideas based on feedback. These DT concepts were further refined and popularized by numerous researchers and practitioners, including McKim (1980), Plattner et al. (2011), and Brown (2019).

The comparison of ST and DT is particularly relevant for animal science modeling as they offer complementary perspectives for model development. Systems thinking provides the framework for understanding complex biological systems and their interactions, while DT ensures models meet practical end-user needs. For instance, in nutrition modeling, ST helps capture complex metabolic interactions, while DT ensures the model remains useful for field nutritionists. Understanding both approaches enables the development of models that are both scientifically robust and practically applicable.

These logical thinking methodologies have some key differences. While ST focuses on understanding the relationships and interactions within a system, considering the complexity of the system and how different parts influence the whole, DT focuses on solving a specific user-centered problem through creativity and innovation, often in a more localized and immediate context. While ST takes a top-down view of problems, identifying how changes in one part of the system can ripple through the entire structure, DT uses a bottom-up approach, starting from the user's experience and needs, and building towards a solution. Systems thinking looks at the long-term impact of decisions and how they affect the entire system, including unintended consequences. In contrast, DT concentrates more on rapid testing and iterative solutions, refining ideas based on user feedback without necessarily considering broader system-wide consequences in the early stages. Therefore, ST is generally used to model and address complex, systemic problems like climate change, organizational structure, or supply chain issues in which multiple interacting factors are at play. Design thinking finds its way in product development, user experience design, and creative problem-solving scenarios, in which understanding user needs is crucial in generating effective solutions. Systems thinking is about understanding complex systems as a whole, while DT is about finding innovative, user-centered solutions to specific problems through an iterative process. That is the reason that DT has been frequently used in developing capstone courses in which students identify a problem (usually referred to as an ill-defined, ill-structured, or wicked problem) and then identify and evaluate possible solutions to resolve the problem (Donaldson and Smith, 2017).

## 2.1. Application of ST and DT

### 2.1.1. Whole system vs. specific problem

To emphasize the distinction between modeling a whole system versus a specific problem, we consider the well-documented problem of decreasing feed efficiency in a dairy herd. Systems thinking would



look at the entire feeding system and management practices and would consider factors like the quality and type of feed, animal genetics, rumen health, environmental conditions, water availability, herd management practices, and even the economic constraints of the farm. The solution could involve analyzing the interaction among diet composition, herd genetics for feed efficiency, and farm management strategies and adjusting these interrelated factors to optimize feed utilization and milk production. Design thinking would focus specifically on farmers' experiences with feeding practices. It might involve interviewing farmers and nutritionists to understand their challenges with feed preparation and the feeding process or understanding feed data. The solution could involve designing a more user-friendly mobile app to help farmers track feed intake, monitor cow health, or receive suggestions for diet adjustments based on real-time data. The focus would be on making the feeding process more efficient and user-friendly for the farm operator.

Another example is when different space perspectives related to the decline in genetic diversity in a pig breeding program are explored, ST would consider the entire breeding program and its impact on the genetic pool. It would look at the interplay between genetic selection for specific traits (e.g., growth rate, meat quality), the reproductive strategy, and the maintenance of genetic diversity. The solution might involve implementing broader genetic selection criteria, utilizing crossbreeding programs, and managing inbreeding to ensure a sustainable balance between genetic improvement and diversity in the long term. Design thinking would focus on the breeders' experiences and needs regarding maintaining genetic diversity. After interviews, it might reveal that breeders find it difficult to access information on genetic relationships or diversity metrics. The solution could involve developing an intuitive app or tool that helps breeders track genetic diversity in their herds and provides guidelines on which animals to breed to avoid inbreeding, solving the immediate need for more accessible breeding data.

### 2.1.2. Top-down vs. bottom-up modeling approaches

Here, we consider applying top-down and bottom-up approaches to the problem of high calf mortality rates in a beef cattle operation. Systems thinking would take a top-down approach, considering the entire management system that impacts calf health. It would analyze factors like breeding practices, cow health during pregnancy, calving environment, colostrum management, nutrition of both the dam and calf, disease prevention protocols, and weather conditions. The solution might involve implementing more structured breeding programs, improving maternal nutrition, or changing calving protocols, taking into account how these changes interact to improve overall calf survival rates. Design thinking would use a bottom-up approach by starting with calf caregivers' experiences on the farm. Interviews and observations might reveal that caregivers struggle with early calf care, such as ensuring timely colostrum intake. A possible solution might be developing a simple tool or wearable technology that alerts caregivers when a calf has not received colostrum or shows signs of distress. The focus would be on solving immediate problems that caregivers face to reduce calf mortality.

### 2.1.3. Long-term systemic impact vs. short-term problem resolution

Regarding the different time perspectives for the problem of slow genetic progress in a sheep breeding program for parasite resistance, ST would look at the entire breeding system, including genetic selection, nutrition, parasite control, and environmental conditions. It would consider how management practices and genetic diversity are influencing the long-term success of the program. The solution could involve developing a multi-year breeding plan that integrates genetic selection for parasite resistance with improved pasture management and strategic deworming practices, ensuring the sustainability of the flock's health and genetics over time. On the other hand, DT would focus on the immediate problem of parasite resistance. The team might talk to breeders to understand their specific struggles with identifying resistant sheep and managing breeding records. The solution could involve designing a simple genetic selection tool based on current knowledge and models that helps farmers quickly identify parasite-resistant animals based on visual or performance indicators, providing immediate

benefits in genetic progress and parasite management without requiring complex system-wide changes.

Another example regards the difference in sustainable innovation for the problem of reducing methane emissions from ruminants to meet environmental regulations. Systems thinking would consider the entire farm ecosystem, including the types of feed, grazing management, herd genetics, manure management, and environmental regulations. The solution might involve integrating various strategies such as altering feed composition, implementing rotational grazing, selecting low-emission genetics, and improving manure management practices. By looking at the entire system, ST would ensure that methane reduction strategies are sustainable and aligned with both economic and environmental goals over the long term. However, DT would focus on how farmers experience and manage emissions. After engaging with farmers, the design team might discover that farmers find monitoring and tracking methane emissions challenging. A solution could involve creating a simple tool or sensor that helps farmers monitor methane output from their animals in real-time. The focus would be on designing a user-friendly, easy-to-implement system that helps farmers make immediate adjustments to reduce emissions.

#### 2.1.4. Complex systemic problems vs. user-centered problems

Regarding the different applications for the problem of declining fertility rates in dairy cows, ST would consider the entire production system, including genetics, nutrition, environment, heat stress management, cow comfort, and reproductive management. It would explore how changes in nutrition, housing conditions, and herd management interact with fertility. The solution might involve optimizing nutrition (with a particular focus on energy balance), improving cow comfort through better housing and cooling systems, and refining reproductive management strategies, all while considering their long-term effects on fertility rates. Design thinking would focus on improving farmers' ability to manage fertility. After engaging with farmers, the team might discover that they struggle with tracking reproductive cycles and managing heat detection. The solution could be designing an easy-to-use fertility tracking system or wearable technology that alerts farmers when cows are in heat. This user-centered tool would solve the immediate problem of identifying cows ready for breeding without necessarily addressing the broader system issues affecting fertility.

In essence, ST addresses problems by looking at the entire system, including how various factors interact over the long term. In contrast, DT focuses on solving specific user-centered challenges through empathy, rapid iteration, and practical solutions. When modeling a problem, ST may also use expert options to create the CLD of the variables, and often, group modeling techniques are employed with ST. Both approaches offer valuable perspectives and can be used together to create solutions that are both systemic and immediately applicable to stakeholders in the livestock industry.

#### 2.2. Similarities between ST and DT

Indeed, ST and DT can overlap, especially in complex problem-solving situations in which both approaches are needed to generate holistic and innovative solutions. For holistic problem solving, both approaches aim to address complex problems. Systems thinking focuses on understanding the larger system and how various elements interact, while DT emphasizes addressing the needs of users within that system. When combined, they enable problem-solvers to address both the big picture and specific user concerns. Both approaches are iterative in nature. While DT explicitly promotes an iterative approach through prototyping and testing, ST also involves cycles of learning and feedback. Both approaches recognize that solutions are not static, and continuous refinement is needed as new insights are gained. For the interconnectedness in DT, especially when solving complex problems, understanding how different stakeholders, processes, and environments interact (a key concept in ST) is crucial. Design thinking may incorporate ST to ensure that interconnections and dependencies between different system components are considered when designing a solution. For the user-centered systems, DT emphasizes empathy and user needs, but these users often exist within larger systems

(organizations, societies, ecosystems). Systems thinking helps ensure that the context in which the user operates is not overlooked, ensuring that solutions are sustainable and viable within the system. Both approaches can converge when working on sustainable innovation. Systems thinking helps identify potential long-term impacts of decisions on a system-wide level, while DT can guide the creation of solutions that are both innovative and user-centered, ensuring that they are adopted effectively within the system. For a multidisciplinary approach, both DT and ST encourage cross-disciplinary collaboration. Systems thinking calls for experts across various fields to analyze systems from different perspectives, while DT encourages diverse teams to bring creativity to the ideation and prototyping phases. This multidisciplinary collaboration fosters innovative solutions that are both functional within a system and tailored to user needs. For feedback and adaptation, the focus of ST on feedback loops and how changes in one area affect others parallels the feedback of DT from prototypes and testing. Both approaches rely on understanding how real-world interactions (within the system or with users) influence outcomes, leading to adaptation and refinement of ideas.

Though ST and DT have distinct focuses—one on understanding and optimizing complex systems and the other on creativity and user-centric innovation—they are complementary. Together, they provide a more comprehensive approach to problem-solving, ensuring that solutions are both innovative and systemically viable.

### 3. Developing the conceptual model

In the diverse and often complex realm of applied sciences, the development of accurate and insightful models is crucial for understanding multifaceted systems and optimizing research strategies. Visual aids serve as indispensable tools in this process, offering researchers powerful means to conceptualize, analyze, and communicate intricate relationships and dynamics within various scientific domains. The most commonly employed visual aids are CLD, stock and flow diagrams (SFD), mind maps, flowcharts, and concept maps. Each of these tools brings unique strengths to the modeling process, from elucidating feedback mechanisms and quantitative flows to organizing hierarchical information and mapping decision processes. By leveraging these visual techniques, researchers across different scientific disciplines can enhance their ability to identify critical variables, understand system behaviors, and develop more robust and comprehensive models. This integrated approach to visual modeling not only facilitates more profound insights into complex systems but also promotes more effective communication among researchers, stakeholders, and practitioners across various fields of applied science.

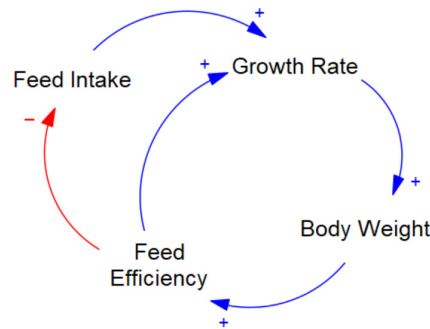
#### 3.1. Causal loop diagrams

Causal loop diagrams serve as a fundamental tool in ST, offering a method to visualize the structure of complex systems by illustrating causal relationships between variables. The primary function of CLD is to elucidate feedback loops within a system, which can be classified as either reinforcing (positive) or balancing (negative). Zinovyev (2015) emphasized the importance of using data visualization in complex systems, in which graphical representations such as CLD help make system behaviors more understandable by revealing these reinforcing and balancing loops. Visualization in this form allows researchers to not only identify causal relationships but also explore the system dynamics more intuitively. The development of a CLD follows a systematic process. Initially, the key variables within the system are identified and listed. Subsequently, arrows are drawn between these variables to represent causal relationships. These arrows are then labeled with either a positive (+) or negative (−) sign, indicating whether the change in the causal variable induces a change in the same or opposite direction in the affected variable, respectively. The next step involves the identification and labeling of feedback loops, denoted as ‘R’ for reinforcing loops and ‘B’ for balancing loops. The final stage is the analysis of the completed diagram to gain insights into the behavior of the system.

To illustrate this concept, consider a CLD representing pig growth and feed efficiency (Figure 1). In this model, “Feed intake” is positively correlated with “Growth rate” and “Body weight.” As “Body



weight” increases, it initially enhances “Feed efficiency,” defined as the conversion of feed to body mass. However, a negative feedback loop emerges as “Body weight” continues to increase, eventually leading to a reduction in “Feed intake.” Concurrently, “Feed efficiency” positively influences “Growth rate,” creating a reinforcing loop within the system.



**Figure 1** - A generalized causal loop diagram of pig growth and feed efficiency.

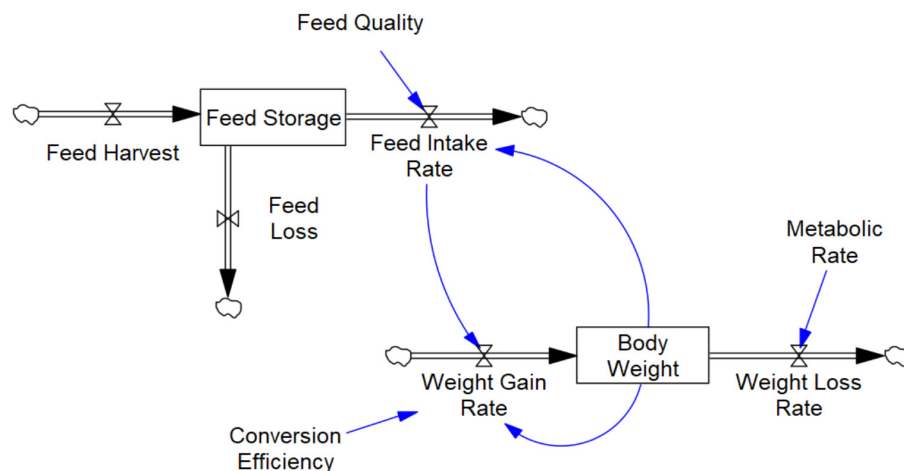
### 3.2. Stock and flow diagrams

Stock and flow diagrams is believed to represent an evolution from CLD, providing a more quantitative representation of system dynamics. These diagrams are particularly adept at illustrating the accumulation and depletion of resources over time. In an SFD, stocks (represented by rectangles) denote accumulations within the system, while flows (depicted as pipes with valves) represent the rates of change in these stocks. Additional elements, called converters (illustrated or not as circles), represent factors that influence the flows. The construction of an SFD begins with the identification of key stocks in the system. Subsequently, the inflows and outflows for each stock are determined. Converters are then added to represent factors influencing these flows. The final steps involve connecting these elements with arrows to show relationships and defining mathematical equations for flows and converters.

The SFD for the pig growth model illustrates the complex interplay of factors influencing pig growth and feed management (Figure 2). At its core, the system revolves around two key stocks: “Feed storage” and “Body weight”. These stocks represent the accumulation of feed inventory and pig mass, respectively, and are subject to various inflows and outflows that drive the dynamics of the system. “Feed storage” is replenished through the “Feed harvest” flow, representing the addition of new feed to the system. Simultaneously, it is depleted by two outflows: “Feed intake rate”, which represents consumption by the pigs, and “Feed loss”, accounting for spoilage or waste. The “Feed intake rate” serves as the primary link between “Feed storage” and “Body weight”, embodying the process of nutrition and growth. “Body weight”, the second critical stock, increases as a result of the “Feed intake rate” and decreases due to the “Weight loss rate”, which represents the ongoing metabolic processes and energy expenditure of the pig. The interplay between these flows determines the net change in the pig’s mass over time. Several converters modulate these flows, adding nuance to the behavior of the system. “Feed quality” influences the efficiency of the “Feed intake rate”, potentially altering the rate at which feed is consumed and converted to body mass. “Conversion efficiency” plays a crucial role in determining how effectively consumed feed translates into increased “Body weight”. The “Metabolic rate” converter affects the “Weight loss rate”, representing variations in the pig’s energy expenditure. The system incorporates important feedback loops that capture the complex nature of biological growth. “Body weight” exerts an influence on both the “Feed intake rate” and “Conversion efficiency”. As a pig grows, its capacity for feed intake may change, and the efficiency with which it converts feed to body mass may alter, often leading to diminishing returns in growth as the animal matures. These interconnections

create a dynamic system in which changes in one component can have ripple effects throughout the system. For instance, improvements in “Feed quality” might increase the “Feed intake rate”, leading to more rapid “Body weight” gain. However, this growth could, in turn, affect the “Conversion efficiency”, potentially stabilizing the growth rate over time. The balance between “Feed harvest” and “Feed loss” is crucial for maintaining adequate “Feed storage”, which underpins the entire growth process. This balance represents the management aspect of pig farming, in which efficient feed storage and utilization are key to optimal growth outcomes.

In essence, this SFD encapsulates the fundamental dynamics of pig growth, integrating aspects of nutrition, metabolism, and farm management. It provides a framework for understanding how various factors interact to influence pig growth, offering insights that could inform feeding strategies, genetic selection, and overall farm management practices. By representing these complex interactions visually, the SFD serves as a valuable tool for both conceptual understanding and potential quantitative modeling of pig growth processes. A more complicated model can be created if energy intake and a target body weight are added to the model to estimate days on feed.

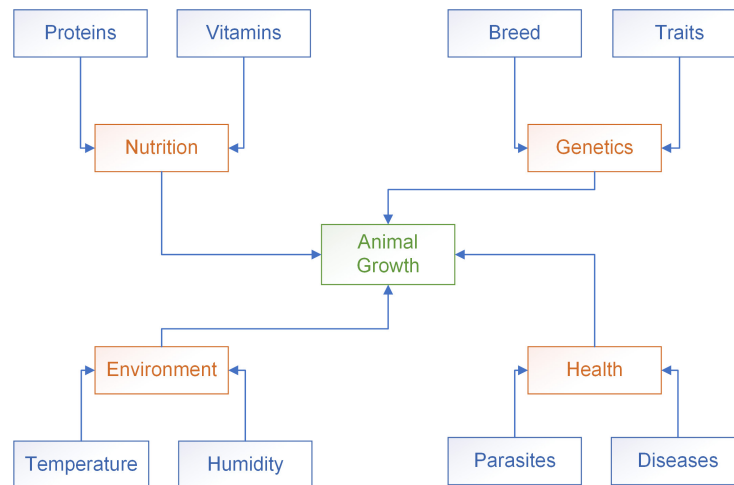


**Figure 2** - A simple stock and flow diagram of pig growth.

### 3.3. Mind maps

Mind maps represent a cognitive tool for visually organizing information, particularly useful in the initial stages of conceptual model development. Unlike CLD and SFD, which focus on system dynamics, mind maps emphasize hierarchical relationships and associations between concepts. The creation of a mind map begins with the central concept placed at the center of the diagram. From this central node, main categories branch outward, with subcategories and details extending from these primary branches. This hierarchical structure allows for the organization of complex information in a visually intuitive manner.

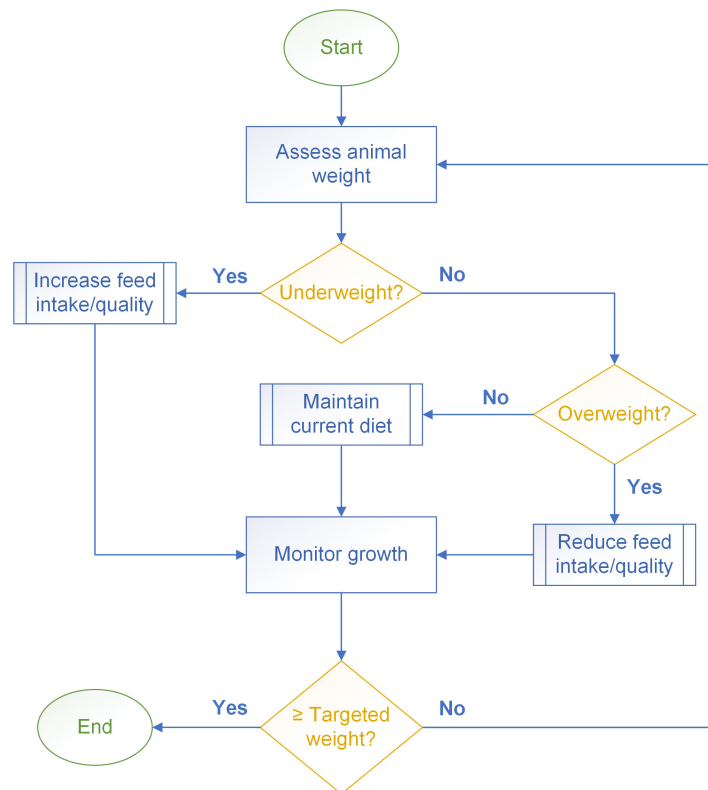
In the context of animal nutrition, a mind map might begin with “factors affecting pig growth” as the central concept (Figure 3). Primary branches could include categories such as nutrition, genetics, environment, and health. Each of these branches would then extend to more specific factors. For instance, the nutrition branch might be further divided into protein content, energy density, mineral balance, and feeding schedule.



**Figure 3** - A mind map of some factors affecting animal growth.

### 3.4. Flowcharts

Flowcharts represent another valuable visual aid in the conceptual modeling process, particularly useful for mapping out processes or decision trees within a system. In the context of animal nutrition, flowcharts can effectively illustrate feeding protocols, diagnostic procedures, or experimental designs. The construction of a flowchart adheres to a standardized set of symbols and conventions (Figure 4). Rectangles typically represent processes or actions, while diamonds indicate decision points or branching paths. Arrows connect these elements, showing the flow or sequence of the process.



**Figure 4** - A flowchart of an animal feeding decision process to achieve a targeted weight.

The development of a flowchart begins with identifying the start and end points of the process. Subsequently, each step or decision in the process is systematically added and connected by arrows to show the progression and potential branching paths.

Consider, for example, a flowchart depicting a basic feeding protocol for growing pigs (Figure 4). The flowchart begins with “Start” and leads to “Assess animal condition”. From this point, a diamond-shaped decision node asks, “Is the pig underweight?” If yes, the path leads to “Increase feed ration”, followed by “Monitor growth”. If no, another decision node asks, “Is the pig overweight?” An affirmative response leads to “Reduce feed ration”, while a negative response results in “Maintain current diet”. All paths eventually converge on “Monitor growth” before cycling back to “Assess animal condition” or proceeding to “End” if the growth phase is complete, i.e., a targetted weight is reached. This flowchart provides a clear visual representation of the decision-making process involved in managing pig feeding regimens. It allows for the quick identification of key decision points and the resulting actions, facilitating both the implementation of the protocol and its communication with other stakeholders.

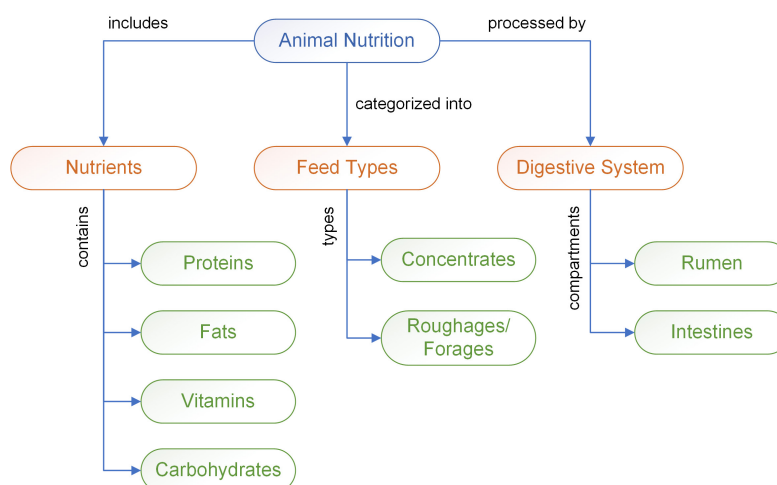
### 3.5. Concept maps

Concept maps serve as a cognitive tool for organizing and representing knowledge, bearing some similarities to mind maps but with distinct characteristics and applications. While mind maps typically branch out from a central concept in a radial structure, concept maps allow for a more flexible arrangement of ideas and explicitly labeled relationships between concepts.

The development of a concept map begins with the identification of key concepts related to the subject matter. These concepts are then arranged hierarchically, with the most general, inclusive concepts at the top and more specific concepts nested below. The critical feature of concept maps is the use of labeled lines or arrows to connect related concepts, with the labels explaining the nature of the relationship between the connected ideas.

In the field of animal nutrition, a concept map might explore the factors influencing feed efficiency in livestock (Figure 5). Animal nutrition is a complex field that encompasses several interconnected concepts. At its core, animal nutrition focuses on three main areas: nutrients, feed types, and the digestive system. Nutrients form the foundation of animal nutrition, including proteins, carbohydrates, fats, and vitamins, each playing a crucial role in an animal’s health and growth. These various nutrient types work together to support different bodily functions and maintain overall welfare. Feed types are another critical aspect of animal nutrition that can be broadly categorized into two main groups: roughages and concentrates. Roughages, such as hay and grass, are high in fiber and form a significant part of many animals’ diets, particularly for ruminants like cattle and sheep. Concentrates, on the other hand, are more energy-dense feeds, often used to supplement an animal’s diet with additional nutrients or to meet higher energy requirements. The digestive system is the third key component in animal nutrition. It processes the consumed feed, breaking down complex nutrients into forms that the animal’s body can absorb and utilize. The efficiency of this system greatly influences how well an animal can extract nutrients from its feed. These three main concepts—nutrients, feed types, and the digestive system—are intricately linked, showing how the nutrients an animal requires influence the types of feed it should consume. The feed types, in turn, affect how the digestive system processes the food. Furthermore, the capabilities of the digestive system determine how effectively the animal can extract nutrients from different feed types. Understanding these relationships is crucial for optimizing animal nutrition. By balancing the proper nutrients, selecting appropriate feed types, and considering the animal’s digestive capabilities, nutritionists and farmers can ensure that animals receive the best possible diet for their health, growth, and productivity.

The strength of concept maps lies in their ability to explicitly show the relationships between different ideas within a complex system. This makes them particularly useful for identifying knowledge gaps, integrating new information with existing knowledge, and fostering a deeper understanding of the interconnections within a field of study.



**Figure 5** - A concept map of animal nutrition.

The application of these visual aids (e.g., CLD, SFD, mind maps, flowcharts, concepts maps) provides researchers in animal nutrition with a diverse toolkit for conceptual modeling. Each technique offers unique advantages: CLD excel in illustrating system dynamics and feedback loops; SFD provide a framework for quantitative modeling; mind maps facilitate brainstorming and hierarchical organization of ideas; flowcharts clearly depict processes and decision points; and concept maps elucidate the complex relationships between concepts within a knowledge domain.

By judiciously employing these visual aids, researchers can develop more comprehensive and nuanced conceptual models. This, in turn, leads to an improved understanding of complex systems in animal nutrition, more effective communication of ideas among researchers and stakeholders, and the development of more accurate and insightful computational models. The choice of which visual aid to use depends on the specific needs of the research question, the complexity of the system under study, and the intended audience for the model.

#### 4. Developing the mathematical model

With our CLD, mind map, or conceptual map in hand, we then translate these ideas into the language of mathematics. This mathematical formulation is where abstract concepts take on concrete form through equations and formulas. It is a creative process requiring us to find suitable mathematical structures to represent the relationships we have identified.

Tedeschi (2023b) contended that as models grow more complex to represent intricate systems better, fully understanding all the interrelationships within the model becomes increasingly difficult. This complexity not only complicates the interpretation but also renders the processes of parameterization, verification, and validation more challenging, as noted by Oreskes et al. (1994), who argued that full validation of complex models is impossible. As the complexity of models increases, so does the number of needed validation cases and the potential for errors in evaluation, which can hinder the practical usability of the model. Burnham and Anderson (2002) emphasize that adding complexity does not always result in better models and suggest that simpler models, which balance complexity and performance, often prove more reliable and interpretable. Tedeschi (2023b) similarly warned that overly complicated models risk becoming too cumbersome for real-world applications, making it harder for scientists and practitioners to utilize them effectively. Therefore, while complexity is sometimes necessary to capture the full scope of a system, it must be balanced with usability to ensure



the model remains functional and not overly burdensome. Swannack et al. (2025) further underscored the significance of good coding practices as integral to good modeling practices, particularly for ecological systems. They advocate for incorporating pseudocode and annotations early in the modeling process to bridge gaps between conceptual understanding and functional code, a practice that is equally applicable to animal science modeling.

These mathematical structures are sometimes pre-determined, with modelers often preferring to use well-established relationships among known variables rather than creating entirely new mathematical structures. This approach ensures that models remain grounded in proven methodologies, which can simplify the processes of validation, parameterization, and communication. As Grimm et al. (2006) pointed out, the use of standardized modeling practices can help enhance the transparency and reproducibility of models, making them more accessible to other researchers and practitioners. However, while pre-determined mathematical structures offer a reliable framework, they may also limit the flexibility needed to capture novel or unique dynamics within a system. Striking a balance between relying on established mathematical tools and innovating new ones is crucial for ensuring that models can both maintain usability and effectively reflect the complexity of the systems they represent.

#### 4.1. Mathematical structures in modeling: Balancing tradition and innovation

In the realm of MM, we often find ourselves at a crossroads between leveraging well-established mathematical structures and forging new paths with innovative formulations. This tension is at the heart of model development, influencing how we represent relationships within complex systems. Many fields have developed a set of “go-to” mathematical relationships that have proven useful over time. These pre-existing formulations offer a tempting starting point for modelers, providing a familiar framework that has been vetted by years of use and scrutiny. However, this reliance on established structures can be a double-edged sword. Consider, for instance, the field of enzyme kinetics. The Michaelis-Menten equation has long been the cornerstone of modeling enzyme-catalyzed reactions. Its ubiquity in the field is a testament to its utility, but it also raises important questions about the limitations it might impose on our understanding. The Michaelis-Menten equation, in its simplest form, is expressed as:

$$v = \frac{v_{max} \times [S]}{K_m + [S]}, \quad [1]$$

in which  $v$  is the reaction rate,  $v_{max}$  is the maximum rate,  $[S]$  is the substrate concentration, and  $K_m$  is the Michaelis-Menten constant.

This equation assumes a simple, single-substrate reaction operating under steady-state conditions. While it has proven invaluable in many contexts, it may not capture the full complexity of all enzymatic systems. Several studies highlight various situations in which the Michaelis-Menten equation may not accurately describe enzyme kinetics, and they propose alternative models or modifications to address these limitations. Some situations in which the Michaelis-Menten model might fall short include multi-substrate reactions, allosteric regulation, cooperativity between enzyme subunits, spatial heterogeneity in cellular environments, and temporal dynamics in rapidly changing systems.

When discussing the limitations of the Michaelis-Menten equation, it is important to note its inability to accurately describe the behavior of cooperative enzymes. As Cárdenas (2013) pointed out, while foundational in enzyme kinetics, the Michaelis-Menten equation fails to capture the complex behavior exhibited by cooperative enzymes. This limitation has led researchers to develop more comprehensive models. Cárdenas (2013) provided a historical perspective on this issue, tracing the long road from the initial formulation of the Michaelis-Menten equation to the recognition and modeling of cooperativity. This work highlights how the simple hyperbolic kinetics described by the Michaelis-Menten equation are insufficient for explaining the sigmoidal curves often observed with cooperative enzymes. Building on this understanding, researchers have worked to develop generalized models that can describe both cooperative and non-cooperative kinetics. For instance, Schnell and Maini (2000) proposed

more general models that account for enzyme behavior at high enzyme concentrations, a condition in which the Michaelis-Menten equation often fails. Their work provides mathematical frameworks that can be applied to both cooperative and non-cooperative systems, offering a more versatile approach to enzyme kinetics modeling. Grima (2009) showed that the Michaelis-Menten equation can give incorrect results in situations with low molecule numbers or spatial heterogeneities, which are common in living cells. Hanson and Schnell (2008) demonstrated that the steady-state assumption of the Michaelis-Menten equation does not hold for rapid enzyme reactions, leading to significant errors in rate predictions. Cornish-Bowden (2015) discussed how the Michaelis-Menten equation is often insufficient for multi-substrate, multi-product enzyme reactions, highlighting the need for more complex kinetic models to describe these systems accurately. English et al. (2006) demonstrated that single-enzyme experiments reveal complex fluctuations in catalytic rates that are not captured by the classical Michaelis-Menten equation. Qian (2012) showed that the Michaelis-Menten equation needs to be modified for enzyme reactions maintained in non-equilibrium steady states to account for the chemical driving force. The question arises: Do we need to use the Michaelis-Menten equation in all cases? The answer is a resounding no. In fact, mindlessly applying this or any pre-established formulation without considering alternatives can limit our ability to accurately represent and understand complex biological systems.

Alternative approaches to enzyme kinetics modeling might include power-law formulations (e.g., the Hill equation for cooperative binding; Hill, 1910), stochastic models that account for randomness in molecular interactions, spatial models that incorporate diffusion and compartmentalization, and machine learning approaches that can capture complex, nonlinear relationships without assuming a specific functional form. The impact of choosing an alternative formulation can be significant in numerical simulations. While the differences might be subtle in some cases, in others, they could lead to qualitatively different predictions. For example, a model incorporating cooperativity might predict a much sharper transition in enzyme activity in response to substrate concentration compared to the gradual saturation curve of the Michaelis-Menten model.

Moreover, the choice of mathematical structure can influence not just the quantitative predictions of a model but also our conceptual understanding of the system. A different formulation might highlight aspects of the system that were obscured by the assumptions inherent in more traditional approaches. This is not to say that we should abandon well-established mathematical structures altogether. Instead, we should approach them with a critical eye, constantly asking ourselves four questions: What assumptions are built into this formulation? Do these assumptions hold for the specific problem the modeler is studying? What aspects of the problem might this formulation fail to capture? Are there alternative approaches that might provide new insights?

By maintaining this balance between leveraging established knowledge and exploring new mathematical terrain, we can develop models that are both grounded in solid principles and capable of capturing the full complexity of the systems we study. This approach not only leads to more accurate and insightful models but also drives the field forward, pushing the boundaries of our mathematical and conceptual understanding.

#### 4.2. Advanced mathematical techniques in model development

Several sophisticated mathematical techniques have proven valuable in addressing the complexity of animal science models. Singular perturbation methods, particularly useful in multi-scale biological systems, help separate fast and slow processes in animal metabolism and growth models. For instance, these methods can distinguish between rapid enzymatic reactions and slower physiological adaptations in ruminant digestion models.

Singular value decomposition (SVD) offers powerful tools for analyzing complex datasets and reducing model dimensionality while preserving essential relationships. In animal nutrition studies, SVD can help identify key patterns in feed intake and growth data, enabling more efficient model parameterization. Alter et al. (2000) applied SVD in genome-wide expression data to demonstrate

its power in transforming complex biological data into interpretable patterns, revealing hidden relationships between genes and experimental conditions. Similar approaches could be valuable in animal nutrition for uncovering patterns in large-scale feeding and growth datasets.

Model identifiability analysis, crucial for ensuring reliable parameter estimation, determines whether unique parameter values can be determined from available experimental data (Muñoz-Tamayo and Tedeschi, 2023). This is particularly relevant in animal nutrition models in which multiple parameters often interact to produce observed outcomes. For example, in models of ruminant methane production, identifiability analysis helps determine which emission factors can be reliably estimated from typical measurement protocols.

Hybrid modeling approaches, combining mechanistic and empirical elements, have emerged as powerful tools for capturing complex biological processes (Tedeschi, 2019; Tedeschi, 2023b). These approaches are particularly valuable in animal science, in which some processes (like basic metabolism) are well-understood mechanistically, while others (like individual animal behavior) may be better represented empirically. For instance, hybrid models of dairy cow performance might combine mechanistic representations of rumen function with empirical relationships for feed intake behavior.

In the end, the goal of MM is not just to describe what we already know, but to reveal what we have yet to discover. By being open to new mathematical structures and constantly questioning our assumptions, we create the potential for breakthrough insights that can reshape our understanding of complex systems.

#### 4.3. Programming mathematical models: Ensuring connectivity and future compatibility

Implementing mathematical models in computer code is a distinctive step in the modeling process that can significantly impact the usefulness, longevity, and ability of the model to integrate with other models. Concern about the challenges of incorporating older models (i.e., legacy models) into new ones without extensive rewriting is well-founded and reflects a common issue in the field. Recent work by Swannack et al. (2025), examining the challenges faced by ecological modelers, emphasized that proper documentation, modular design, and clean coding practices are essential for developing sustainable scientific software. Their pedagogical findings highlight how early adoption of these practices can prevent many common implementation issues. There are many more challenges with “legacy models”, including proprietary software with limited export capabilities, outdated programming languages, highly specialized and domain-specific languages, poor documentation practices, and hardcoded parameters and inflexible structures. These factors often result in models that are difficult to maintain, update, or integrate into larger systems. The need to completely rewrite these models not only introduces the risk of new bugs but also requires significant time and resources.

In the ever-evolving landscape of scientific modeling, researchers often find themselves standing at a crossroads between the familiar terrain of established models and the uncharted territory of new methodologies. This journey is not just about the mathematics behind the models but also about how we bring these models to life through computer code.

As we look back on the path we have traveled, we can see the remnants of models past—legacy code written in now-obsolete languages, or worse, locked behind proprietary software, trapped in outdated operating systems and deprecated programming languages. For example, early ruminant nutrition computer models were developed using languages or programs that are now extinct or being phased out. Several versions of the mathematical models of lactating dairy cows developed by R. Lee Baldwin and colleagues (Baldwin, 2008; France, 2013)—such as *Cow*, *Myrtle*, *Daisy*, and *Molly*—were written in the Advanced Continuous Simulation Language (ACSL), developed in the mid-1970s (Mitchell and Gauthier, 1976). Similarly, the first electronic version of the Cornell Net Carbohydrate and Protein System (CNCPS) was programmed using a Lotus 1-2-3 spreadsheet (Fox et al., 1990; Tedeschi and Fox, 2020). Notably, the very first desktop version, developed by Danny Fox and Charlie Sniffen in 1979,

used a TRS-80 computer. Notwithstanding their age and the deprecated programming languages used to develop these models, there have been several efforts to update and refine the original systems (Fox et al., 2004; Gregorini et al., 2013; Tedeschi and Fox, 2020; Tylutki et al., 2008; Van Amburgh et al., 2015), some of which are commercialized today. However, they are not entirely available to the public, limiting independent development and verification. This poses significant challenges for researchers and developers seeking to test or improve upon these foundational models. Therefore, while valuable, these relics of our scientific history often resist integration into the modern modeling ecosystem. Researchers like Anzt et al. (2021) have highlighted this challenge, noting how outdated or closed-source software can impede scientific progress and reproducibility. A modular design approach is preferable because models are treated as a collection of interconnected modules rather than monolithic scripts and object-oriented programming principles to create reusable components.

Consider, for instance, the field of climate modeling. In the early days, models were often developed as monolithic structures, tightly coupled to specific computing environments. The Earth System Modeling Framework (ESMF), introduced by Hill et al. (2004), emerged as a response to this challenge. It provided a standardized way to couple different components of climate models, allowing atmosphere, ocean, and land models to communicate seamlessly. This framework exemplifies the shift towards modular, interoperable model design that we now recognize as crucial for sustainable scientific software.

Nevertheless, the journey does not end with modular design. As we forge ahead, we increasingly recognize the value of open-source, general-purpose programming languages. With its rich ecosystem of scientific libraries like NumPy and SciPy, Python has become a lingua franca in many scientific domains. Its rise in scientific computing, as chronicled by Millman and Aivazis (2011), is a testament to the power of community-driven, open-source development in advancing scientific modeling. Using open-source, general-purpose languages like Python, R, or Julia has broad community support, extensive libraries, continuous updates, fixes, and improvements, and better interoperability with other systems.

Yet, even as we embrace these new tools, we must be mindful of the pitfalls that await the unwary traveler. Hardcoded parameters, poorly documented functions, limited speed typically caused by implementation inefficiencies and lack of algorithmic or data scalability, and brittle dependencies can turn today's cutting-edge model into tomorrow's maintenance nightmare. This is where practices from the world of software engineering come to our aid. Version control systems like Git, once the domain of software developers, are now essential tools in the scientific modeling toolkit. Perkel (2016) described how these tools are transforming scientific collaboration and reproducibility.

As our models grow in complexity, we are also learning the value of virtual environments such as *pyenv* and *conda* for Python and more generic containerization technologies like Docker. While the creation of virtual environments enables decoupling and isolation of Python installations and associated dependent packages, the containerization tools, as explored by Boettiger (2015), allow us to encapsulate not just our model code but the entire computational environment needed to run it. This approach ensures that our models can travel across different computing landscapes without losing their functionality.

The path forward is illuminated by initiatives that seek to standardize how we represent and share models. The Systems Biology Markup Language (SBML), described by Hucka et al. (2003), offers a common language for representing computational models in systems biology. Similarly, the COMBINE archive format provides a way to package and share models along with their associated data and metadata, addressing the challenge of model reproducibility and reuse.

As we continue this journey, we are seeing the emergence of platforms that embody these principles of openness, modularity, and standardization. The Cell Collective platform, introduced by Helikar et al. (2012), allows researchers to build and analyze computational models through a web-based interface collaboratively. This platform demonstrates how modern approaches to model development can foster a more connected and collaborative scientific community.

Similarly, in the field of system dynamics, the “Molecules” approach developed by Jim Hines for the Vensim environment (Ventana Systems, Inc; <https://vensim.com/>) offers another perspective on modular model building. While confined to a specific software ecosystem, this approach illustrates how, even within proprietary environments, steps can be taken to improve model construction and reusability (<https://vensim.com/modeling-with-molecules-2-02/>).

Looking to the horizon, we can see initiatives like OpenMODEL (<https://open-model.eu/>), which aims to create open, interoperable model components for ecology and environmental sciences. These efforts promise to address many of the integration challenges that have plagued legacy models. Furthermore, platforms like JupyterHub (<https://jupyter.org/hub>) have revolutionized collaborative coding and model development across various scientific disciplines. These environments allow for real-time collaboration, easy sharing of models, and integration of code, documentation, and results in a single interface.

Our journey in mathematical model programming is ongoing, and the landscape continues to evolve. By embracing open-source tools, adopting modular design principles, and committing to standards for model representation and sharing, we are creating a future in which models can be more easily integrated, updated, and built upon. This path, while sometimes challenging, leads us towards a more collaborative, reproducible, and ultimately more impactful scientific modeling practice. By adopting these practices, we can create models that are more robust, easier to maintain, and more readily integrated into larger systems or updated with new findings. This approach saves time, reduces errors in the long run, and promotes a more collaborative and progressive scientific modeling community.

#### 4.4. Data challenges in model parameterization, evaluation, and prediction

However, a model is only as good as the data that informs it. So, the next step is to embark on the crucial task of parameter estimation and data collection. This might involve diving into existing literature, conducting experiments, or consulting experts in the field. It is a phase of calibration in which we fine-tune our model to align with real-world observations. The journey from concept to reliable prediction in MM is fraught with data-related challenges.

##### 4.4.1. Data for model parameterization

Researchers often encounter significant challenges regarding data availability for model parameterization and calibration. Kirchner (2006) captured this dilemma, noting that even the most scientifically rigorous conceptual model becomes ineffective if it cannot be reconciled with empirical data. The crux of the issue lies in the frequent scarcity or complete absence of necessary data, particularly in complex fields such as ecological modeling. Grimm et al. (2014) highlighted this problem in individual-based models, in which many required parameters prove difficult or impossible to measure directly in field conditions. In animal science, a notable gap exists in methane (CH<sub>4</sub>) data for grazing systems, making it particularly difficult to model their impact on greenhouse gas emissions. Tedeschi and Beauchemin (2023) emphasized that the inherent methodological limitations, including discrepancies between bottom-up and top-down approaches, as well as variability in measurement techniques, hinder reliable CH<sub>4</sub> estimates for grazing cattle. This data scarcity mirrors broader challenges in modeling nutrition for grazing animals, underscoring the critical need for robust models that accommodate these complexities.

Faced with this data deficit, modelers often resort to alternative methods for parameterization. These may include relying on indirect measurements, imputing missing values, drawing from literature values, or soliciting expert opinions. While these approaches allow for model development to proceed, they introduce additional layers of uncertainty and errors that must be carefully considered and managed. Researchers have developed several strategies to increase model robustness to address these data-related challenges. As described by Saltelli et al. (2007), sensitivity analysis serves as a valuable tool for identifying the parameters that most significantly influence model outcomes. This approach allows researchers to prioritize their data collection efforts, focusing on these critical parameters to maximize



the impact of limited resources. Bayesian methods offer another powerful approach, as outlined by Cressie et al. (2009). These techniques provide a framework for incorporating prior knowledge and explicitly accounting for uncertainty in parameter estimation, making them particularly useful when dealing with sparse or noisy data. Additionally, meta-analysis techniques, such as those discussed by Gurevitch et al. (2018), enable researchers to synthesize parameter estimates from multiple studies, potentially providing more robust estimates by leveraging the collective knowledge of the field. Moreover, data augmentation techniques have been devised for predictive modeling, in which artificially generated data is created by applying various transformations that minimally alter existing data. These techniques enhance model performance and generalizability, particularly for scarce data ranges, while reducing modeling dependencies on large data sets and mitigating overfitting (Mumuni and Mumuni, 2022).

While not eliminating the fundamental challenge of data scarcity, these methodologies offer modelers a set of tools to navigate the complex landscape of model parameterization and calibration in data-limited scenarios. By employing these techniques, researchers can work towards developing models that, despite data limitations, still offer valuable insights into the systems they aim to represent.

#### 4.4.2. Independent datasets for model evaluation

The ideal model evaluation scenario is to collect independent datasets under similar conditions to those the model is designed to represent. However, achieving this in practice is often challenging. Tedeschi (2006) emphasized that model usefulness should be assessed through its suitability for a particular purpose rather than seeking absolute validation. Oreskes et al. (1994) argued that models can only be evaluated in relative terms by demonstrating that they are not invalid based on available observations. They emphasize that “validation” in an absolute sense is impossible for open natural systems. This aligns with Tedeschi’s (2006) view that the identification and acceptance of a model’s limitations is an essential step towards developing more reliable and accurate models.

To address the challenge of model evaluation, several approaches have been developed and refined over time. Cross-validation techniques (Efron, 1979, 2003), as described by Arlot and Celisse (2010), involve partitioning a single dataset into subsets for training and testing. This method allows for efficient use of limited data by using different portions for model development and evaluation. Holdout methods, discussed by Kohavi (1995), take a similar approach but set aside a specific portion of available data solely for evaluation, ensuring it is not used in model development or calibration. When truly independent datasets are unavailable, Dietze (2017) suggested using out-of-sample predictions to assess model performance, which can provide insights into how well the model generalizes to new data.

Tedeschi (2006) built upon these approaches, suggesting a more comprehensive strategy for model evaluation and advocating for using a combination of several statistical analyses rather than relying on a single method. This multifaceted approach includes techniques such as analysis of linear regression (though he cautions about its limitations in model evaluation), mean square error of prediction and its decomposition, concordance correlation coefficient, and nonparametric analyses. By employing multiple methods, researchers can gain a more nuanced understanding of model adequacy, considering both accuracy and precision. Furthermore, Tedeschi (2006) highlighted the importance of understanding Type I errors (rejecting a valid model) and Type II errors (accepting an invalid model) in model evaluation. This understanding can guide researchers in designing more robust evaluation procedures and interpreting results more effectively. By considering these potential errors, modelers can better assess the reliability and applicability of their models in different contexts.

In essence, the process of model evaluation is complex and multifaceted, requiring careful consideration of data availability, statistical techniques, and potential sources of error. By integrating insights from various researchers and employing a range of evaluation methods, modelers can work towards developing more robust, reliable, and valuable models that effectively represent the systems they aim to study.

#### 4.4.3. Assessing predictive capabilities

Evaluating the ability of a model to make future predictions is perhaps the most challenging aspect, as it inherently involves unknowns. As Box (1976) stated, “all models are wrong, but some are useful”. This insight underscores the importance of developing robust approaches to assess predictive capabilities. Several methods have been developed to address this challenge. Hindcasting, as described by Hazen et al. (2018), involves using the model to predict past events not used in model development and then comparing these predictions with historical data. This approach provides a way to test the model against known outcomes, offering insights into its predictive accuracy. Ensemble modeling, discussed by Araújo and New (2007) and Tedeschi (2023a), combines predictions from multiple models to assess the range of possible outcomes and associated uncertainties. This method provides a more comprehensive view of potential future scenarios and helps to mitigate the biases or limitations of individual models. Scenario analysis, as outlined by Mahmoud et al. (2009), involves applying the model to a range of possible future scenarios to understand its behavior under different conditions. This technique is instrumental in fields in which future conditions may differ significantly from current or historical conditions. Urban et al. (2016) described the continuous model-data comparison approach, which involves ongoing evaluation of model predictions against new data as they become available. This iterative process allows for model refinement over time, ensuring that the model remains relevant and accurate as our understanding of the system evolves.

It is crucial to remember that model evaluation is not a one-time event but an ongoing process. As new data become available and our understanding of systems evolves, models must be reassessed and refined. Moreover, the appropriate methods for model evaluation and prediction assessment can vary significantly depending on the specific field and model type. For instance, Taylor et al. (2012) discussed approaches used in climate modeling, while Woolhouse et al. (2015) and Clements and Hendry (2006) explored methods used in epidemiology and econometrics, respectively.

In summary, while the challenges of data availability, independent evaluation, and predictive assessment are significant, they also drive innovation in modeling methodologies. By acknowledging these limitations and developing strategies to address them, we can create more robust and reliable models, always mindful of the inherent uncertainties and limitations in our predictions.

#### 4.4.4. The peculiar case of machine learning models

In recent years, machine learning (ML) has emerged as a powerful tool in many scientific disciplines. In the context of applied sciences, leveraging ML could reduce the complexity of models without sacrificing predictive power, addressing one of the core challenges traditional modeling approaches face: the balance between simplicity and real-world applicability. The potential for ML to assist with model generation, bug detection, and simulation efficiency presents an opportunity to refine current methodologies and embrace innovation within the field.

However, the development and evaluation of ML models present unique challenges, particularly in fields in which extensive datasets are not readily available. Animal science is a prime example of such a domain, in which the complexity of biological systems and the practical limitations of data collection often result in datasets that are insufficient for traditional ML approaches. The challenge of limited data availability in animal science, particularly in modeling complex biological processes such as methane emissions from ruminants, necessitates innovative approaches to data generation and analysis. Najafabadi et al. (2015) noted that the performance of ML models, especially for deep learning algorithms, often scales with the amount of training data available. This creates a significant hurdle in fields like animal science, in which data collection can be time-consuming, expensive, and constrained by ethical considerations. Furthermore, the inherent biological variability in these systems often requires large sample sizes to capture true patterns effectively. Liakos et al. (2018) reviewed ML applications in agriculture and animal science, highlighting that while ML shows promise, limited data availability often constrains its applicability.

To address these challenges, researchers in animal science and related fields have developed several strategies. Tedeschi (2024) proposed a rank-based method for generating synthetic databases with correlated non-normal multivariate distributions, specifically aimed at enhancing the accuracy and reliability of predictive modeling tools in scenarios with limited data. This approach provides a practical solution for creating realistic, statistically sound datasets when original data is scarce or sensitive. Other techniques that have been employed include transfer learning, as demonstrated by Dórea et al. (2018) in cattle behavior classification. This method adapts models trained on larger datasets from related domains to the specific context of animal science. Data augmentation techniques, such as image rotation or noise addition in computer vision tasks for animal monitoring, have also been utilized to artificially increase the size of training datasets (Neethirajan, 2020).

In the field of animal breeding, Shahinfar et al. (2012) applied artificial neural networks and adaptive neuro-fuzzy inference systems to predict breeding values in dairy cattle, showcasing the potential of these ML approaches in scenarios where data constraints might limit traditional methods. While still emerging in animal science, synthetic data generation techniques have shown potential in other biological fields (Ching et al., 2018). Additionally, federated learning approaches, which allow models to be trained across multiple decentralized datasets without sharing raw data, could be beneficial in collaborative animal science research (Rieke et al., 2020).

The evaluation of ML models in data-limited fields presents its own set of challenges. With limited data, models are prone to overfitting, making rigorous cross-validation techniques even more crucial (Arlot and Celisse, 2010). Concerns about generalizability are paramount, as it is often unclear how well models will perform beyond the limited datasets they are trained on. This necessitates thorough out-of-distribution testing (Dietterich, 2017).

In fields like animal science, model interpretability is often as important as predictive performance. Techniques such as Permutation Feature Importance (Altmann et al., 2010) and SHAP (SHapley Additive exPlanations) can help explain model decisions (Lundberg and Lee, 2017). Furthermore, integrating domain expertise into model evaluation is crucial, as demonstrated by Morota et al. (2018) in their discussion of incorporating biological knowledge in genomic prediction models for animal breeding.

Despite these challenges, the potential of ML in animal science and similar data-limited fields is significant. Progress may come through interdisciplinary collaboration, novel data collection methods leveraging technologies like IoT sensors and automated monitoring systems (Neethirajan, 2020), and the development of hybrid models. Tedeschi (2019) discussed the integration of genomics with nutrition models to improve the prediction of cattle performance and carcass composition under feedlot conditions, demonstrating the potential for combining different modeling approaches. Furthermore, Tedeschi (2023b) highlighted the importance of developing redesigned models that can integrate existing technological advancements in data analytics while taking advantage of accumulated scientific knowledge. This approach could lead to more comprehensive and accurate models in animal science. Open data initiatives within the animal science community could also play a crucial role in building larger, more diverse datasets.

In summary, while the development and evaluation of ML models in data-limited fields like animal science present significant challenges, they also offer opportunities for innovation. By adapting existing ML techniques, developing new approaches tailored to the unique constraints of the field, and fostering interdisciplinary collaboration, researchers can harness the power of ML to drive new insights and advancements in animal science and beyond.

#### 4.5. The art and science of model refinement, evaluation, and application

##### 4.5.1. Model testing and refinement: Walking the tightrope

Once a model is implemented and initially parameterized, we enter a critical phase of testing, optimization, and refinement. This stage is akin to walking a tightrope—we must balance the desire for

model accuracy with the risk of overfitting. While modern computational power has greatly enhanced our ability to handle complex calculations and parameter estimation, the fundamental challenges of model testing and refinement persist. These challenges stem not from computational limitations but from the inherent difficulties in validating model assumptions, ensuring interpretability, and maintaining transparency in model behavior. The process typically begins with verification, ensuring that our implementation accurately reflects our mathematical formulation. As Oberkampf and Roy (2010) emphasized, verification is a purely mathematical exercise, checking that we have correctly solved the equations we have set up.

Next comes the evaluation phase, in which we compare model predictions against real-world data. This often leads to an iterative process of refinement, tweaking equations, or adjusting parameters. Despite advances in artificial intelligence and ML that facilitate parameter optimization, a significant challenge remains: how far should one go in tweaking their models to achieve satisfactory evaluation statistics? Even with powerful computing resources, this question touches on a fundamental issue in model development. As noted by Oreskes et al. (1994), models of open, complex systems can never be truly validated, only evaluated in relative terms. Therefore, the goal of tweaking should not be to achieve perfect agreement with data but rather to improve the representation of key processes of the model while maintaining its generalizability.

Burnham and Anderson (2002) proposed using information criteria, such as Akaike information criterion (AIC) or Bayesian information criterion (BIC), to balance model fit against complexity. These approaches help modelers avoid overfitting by penalizing the addition of extra parameters. Another approach, suggested by Wagener and Gupta (2005), is to use multi-objective evaluation criteria. Instead of tweaking the model to optimize a single metric, modelers can consider multiple aspects of model performance simultaneously, leading to more robust and realistic models.

#### 4.5.2. Uncertainty and sensitivity analysis: Embracing the unknown

As our confidence in the model grows, we delve into uncertainty and sensitivity analysis. This critical phase helps us understand the boundaries of reliability of our model and how changes in inputs or parameters affect our outputs. Saltelli et al. (2007) provided a comprehensive guide to global sensitivity analysis, emphasizing its role in understanding model behavior, calibrating parameters, and prioritizing research and data collection efforts.

Uncertainty analysis, on the other hand, focuses on quantifying the uncertainty in model outputs due to uncertainties in inputs and parameters. Techniques like Monte Carlo simulation, as described by Helton et al. (2006), allow modelers to propagate input uncertainties through their models, providing a range of possible outcomes rather than a single-point estimate. These analyses often reveal surprising aspects of our models. As noted by Oakley and O'Hagan (2004), sensitivity analysis can uncover unexpected relationships between inputs and outputs, leading to new insights about the system being modeled.

#### 4.5.3. Documentation: The unsung hero of modeling

In the development and application of mathematical models, comprehensive documentation plays a crucial role throughout the entire modeling process. Swannack et al. (2025) demonstrated through their teaching experiences that thorough documentation not only facilitates model development and maintenance but also serves as a crucial learning tool for new modelers. Their work showed that maintaining detailed documentation helps modelers track their thought processes, troubleshoot issues, and ensure reproducibility. This practice, as emphasized by Grimm et al. (2014) in their overview of the TRACE (TRANSPARENT and Comprehensive model "Evaluation") framework, is fundamental to ensuring model credibility and reusability. Thorough documentation encompasses recording assumptions, methodologies, successes, and failures, serving multiple essential purposes in the scientific process.

Primarily, documentation provides a means for modelers to track their thought processes and decisions, creating a valuable reference for future work and model refinement. This internal record-keeping is particularly important in complex modeling projects that may span extended periods or involve multiple iterations. Additionally, well-maintained documentation enables other researchers to understand, replicate, and build upon existing work, fostering collaboration and advancing the field as a whole. This aspect of documentation aligns with the principles of reproducible research, a cornerstone of scientific integrity (Peng, 2011).

From a practical standpoint, comprehensive documentation facilitates model maintenance and updates over time. As models evolve to incorporate new data, methodologies, or theoretical insights, clear documentation of previous versions and decision points becomes invaluable. This is especially critical in long-term modeling projects or when models are handed over between different research teams or generations of researchers (Jakeman et al., 2006).

Furthermore, thorough documentation supports model credibility by clearly communicating the scope, limitations, and underlying assumptions of the model. This transparency is essential for stakeholders and decision-makers who may rely on model outputs for policy or management decisions. As noted by Schmolke et al. (2010), clear communication of model assumptions and limitations is crucial for appropriate model use and interpretation in environmental decision-making contexts.

In the field of animal science and nutrition modeling, the importance of documentation has been further emphasized by Tedeschi et al. (2014), who highlighted the need for transparent reporting of model development, evaluation, and application processes. This transparency not only enhances the scientific rigor of modeling efforts but also facilitates the integration of models across different scales and disciplines, a key consideration in addressing complex agricultural and environmental challenges.

#### 4.5.4. Application and continuous improvement: The never-ending cycle

The application of mathematical models in scientific research represents not an endpoint but rather a crucial phase in an ongoing cycle of refinement and discovery. Swannack et al. (2025) observed that one of the biggest challenges for new modelers is transitioning from model conceptualization to implementation while maintaining scientific rigor. Their work suggests that iterative refinement coupled with consistent documentation and testing helps bridge this gap. When a model is deployed to address the questions that initially motivated its development, it often reveals new avenues of inquiry and areas for improvement, thus initiating a new iteration of the modeling process. This cyclical nature of modeling is well-established in the scientific community and forms a cornerstone of the iterative approach to knowledge generation.

Jakeman et al. (2006) articulated this concept through their description of an iterative process encompassing model development, evaluation, and refinement. Their work emphasizes the critical importance of revisiting earlier stages of model development as new information becomes available, highlighting the dynamic nature of model evolution. This perspective aligns with the broader scientific principle of continuous improvement and adaptation in the face of new evidence.

The need for ongoing evaluation and updating of models becomes particularly apparent when they are applied to novel situations or when the underlying systems they represent undergo changes over time. Kelly et al. (2013) explored this phenomenon in the context of ecological forecasting, underscoring the significance of adaptive modeling approaches capable of incorporating new data and knowledge as they emerge. This adaptive capacity is crucial for maintaining model relevance and accuracy in dynamic environmental systems.

In ML and deep learning, various adaptive learning paradigms have been explored, such as online learning (i.e., incremental learning), reinforcement learning, and lifelong learning. Online learning models receive and process data sequentially, typically from a data stream, and are especially



useful when collecting large datasets is time-consuming or when training on an entire dataset is computationally impractical. Within this computational paradigm, each data point or batch of data points is used to update and improve a model iteratively. These models were successfully applied in areas such as predicting user preferences for products (Herbster et al., 2005) and detecting malicious websites (Ma et al., 2009). On the other hand, reinforcement learning (Kaelbling et al., 1996) allows a model to learn through trial-and-error interactions in a dynamically changing environment, diverging from supervised learning since the correct outputs for given inputs are not known in advance. The model receives positive or negative rewards based on interactions and uses this feedback to build a strategy that maximizes rewards over time. However, reinforcement learning typically focuses on a single task and environment without accumulating knowledge to learn future tasks. This paradigm is widely applied across industries, including supply chain management (Rolf et al., 2023), robotics (Singh et al., 2022), and complex industrial optimization problems (Kegyes et al., 2021). In contrast to the single-task focus of online and reinforcement learning, lifelong learning (Chen and Liu, 2017) is a more advanced machine learning paradigm that aims to learn from various tasks, accumulate knowledge, and identify general patterns that help learn new tasks. This approach is effective for tasks that share information and is seen as the next stage of machine learning modeling, in which inductive transfer of information can be used to facilitate learning similar tasks.

Furthermore, the iterative nature of modeling extends beyond mere technical refinement. As noted by Augusiak et al. (2014), the process of model evaluation, or “evaluation” as they term it, is a multifaceted endeavor that includes assessing the underlying conceptual framework of a model, its implementation, and its overall performance. This comprehensive approach to evaluation ensures that models not only improve in their predictive capabilities but also in their theoretical foundations and practical applicability.

In the field of agricultural systems modeling, Jones et al. (2017) emphasized the importance of this continuous improvement cycle in addressing complex challenges such as food security and climate change adaptation. They argue that the development of next-generation models requires not only technical advancements but also improved mechanisms for model integration, data sharing, and stakeholder engagement.

Finally, Tedeschi et al. (2014) provided a concrete example of this iterative process in the context of dairy cattle modeling. Their work on the Agricultural Model Intercomparison and Improvement Project (AgMIP) for livestock demonstrates how the comparison and evaluation of multiple models can drive improvements across the field, leading to more robust and reliable predictions.

In summary, the application of a model marks not the end of the modeling process but rather a critical juncture in an ongoing cycle of refinement, discovery, and adaptation. This cyclical approach ensures that models remain relevant, accurate, and valuable tools for scientific inquiry and decision-making in the face of evolving knowledge and changing systems.

## 5. Conclusions

The development, evaluation, and application of mathematical models is a journey of continuous refinement, creativity, and discovery. Far from being a linear process, modeling requires revisiting and rethinking assumptions, structures, and data as new insights and challenges emerge. Striking a balance between complexity and usability, tradition and innovation, allows us to create models that are not only robust but also accessible and practical for real-world applications. Through this cyclical process of iteration and improvement, we refine our tools, enhance our understanding of complex systems, and drive scientific progress. The ultimate goal is not simply to create accurate models but to push the boundaries of our knowledge, ensuring that these models remain flexible and adaptable as novel discoveries reshape the scientific landscape. This iterative approach leads us towards more reliable, sustainable solutions that address pressing challenges in fields such as animal science and beyond.

## Data availability

Data sharing is not applicable to this article as no data were created or analyzed in this study.

## Author contributions

**Conceptualization:** Tedeschi, L. O. **Investigation:** Tedeschi, L. O. **Methodology:** Tedeschi, L. O. and Tulpan, D. **Supervision:** Tedeschi, L. O. **Writing – original draft:** Tedeschi, L. O. **Writing – review & editing:** Tedeschi, L. O.; Tulpan, D.; Menendez III, H. M. and Vieira, R. A. M.

## Conflict of interest

The authors declare no conflict of interest.

## Acknowledgments

The authors acknowledge partial support of the Texas A&M University Chancellor's Enhancing Development and Generating Excellence in Scholarship (EDGES) Fellowship, the United States Department of Agriculture – National Institute of Food and Agriculture (USDA-NIFA) Hatch Fund (09123): Development of Mathematical Nutrition Models to Assist with Smart Farming and Sustainable Production, and the National Animal Nutrition Program (NANP; <https://animalnutrition.org>), which is a National Research Support Project (NRSP-9) supported by agInnovation, the State Agricultural Experiment Stations, the Natural Resources Conservation Service, and Hatch Funds provided by the National Institute of Food and Agriculture, U.S. Department of Agriculture, Washington, DC.

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