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From Modelling Turbulence to General Systems Modelling

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Abstract: Complex adaptive and evolutionary systems can, at least in principle, be modelled in ways that are similar to modelling of complex mechanical (or physical) systems. While quantitative modelling of turbulent reacting flows has been developed over many decades due to availability of experimental data, modelling of complex evolutionary systems is still in its infancy and has huge potential for further development. This work analyses recent trends, points to the similarity of modelling approaches used in seemingly different areas, and suggests a basic classification for such approaches. Availability of data in the modern computerised world allows us to use tools previously developed in physics and applied mathematics in new domains of scientific inquiry that previously were not amendable by quantitative evaluation and modelling, while raising concerns about the associated ethical and legal issues. While the utility of big data has been repeatedly demonstrated in various practical applications, these applications, as far as we can judge, do not involve the scientific goal of conceptual modelling of emergent collective behaviour in complex evolutionary systems.

Keywords: turbulent combustion modelling; multiscale phenomena; chaotic order; big data; modelling complex systems

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1. Introduction

The remarkable expansion of the internet and computer technologies has brought unprecedented opportunities for accumulating data, implying that hypotheses and theories that previously had purely qualitative characteristics can now be quantified and tested [1]. These changes should bring an extension of methods developed in exact sciences and applied mathematics into areas of scientific enquiry associated with social and other related complex systems. These methods, of course, are not limited to basic statistics and conventional data processing, and they involve a number of different approaches associated with modelling complex systems.

One of the most complex mechanical systems we know is turbulence [2]. Turbulent reacting flows combine the complexity of randomness and coherence with a large number of species and reactions. Modelling turbulent reacting flows was perhaps one of the first attempts of quantitative simulations of a fairly complex system. While these efforts had their successes and failures, they certainly led to the development of advanced modelling tools (recently reviewed in [3]), and some of these tools have generic properties, i.e., can be used to simulate and analyse different complex systems. This conceptual similarity, which is shaped by the nature of complexity, has been occasionally discussed in publications [4]. While the author of this work has introduced and, in cooperation with his colleagues, developed new effective approaches to modelling reacting flows (e.g., conditional methods [3]), which also allow for general systemic applications, this work is not restricted to the consideration of conditional models. We explore a broad scope of conceptual issues associated with modelling complex systems in conditions of emerging revolutionary trends of extending quantified knowledge from mechanical and physical into social and psychological domains. The key impetus for developing conceptual ideas examined here is, perhaps, summarised best by the following quote:

> "The revolution developed from people's attempt to understand disorder—or apparent disorder—in nature, including turbulence in fluids, the erratic flows of epidemics, and the arrhythmic writhing of a heart in the moments before death. These ideas have begun to be applied within the social realm, so now there is use of chaos and complexity theory by social theorists, economists, and people looking at therapies and therapeutic communities."
>
> Antony Bryant [5]

2. The New Age of Data Collection and Its Implications for Modelling Complex Systems

The low cost associated with electronic accumulation and storage of data has created a situation where companies and organisations store virtually all data available to them. While this is, indeed, the simplest and safest policy, it does not automatically make organisations more knowledgeable and/or more efficient. As noted by Eisenhauer [6], large volumes of data can obscure or hide information that is really useful or important. To become useful, data need to be processed and properly categorised. This often requires not only knowledge of data processing and database maintenance but also knowledge of the real world that these data represent.

These trends become even more evident when dealing with data used for the expansion of scientific knowledge and research. On one hand, the availability of data characterising complex social systems opens up, at least in principle, the possibility for the development and validation of new quantitative theories and methodologies in areas which were not previously amenable to quantitative analysis. Numerous methods of applied mathematics can now be used for quantitative analysis in areas that previously could be studied only qualitatively. On the other hand, data are just data, and the formal use of mathematical tools without developing proper physical understanding of the processes can lead to illusory successes. For complex systems, these data are usually represented by a sparse set of points in spaces of extremely large dimensions; these points reflect both systemic dependencies and effects of numerous unpredictable factors that can be seen and treated as random. For such systems, conventional tools of data analysis (such as correlation and principal component analyses) may or may not produce useful results. Indeed, even if we observe a correlation or an apparent dependence between two factors, this, generally, does not mean that one of these factors is caused by another since, for example, this co-dependence might be induced by a third factor that remains undetected. A relationship derived purely from data does not, by itself, represent a scientific theory and, if interpreted as a theory confirmed by these data, can lead us to erroneous conclusions. A rational theory needs to be based on the development of understanding, a reasonable hypothesis, application of logic and analysis, construction of a model, performing simulations, and validation and adjustment of the model in comparison with data from the real world. Although important, data are just one of many components needed for creating knowledge. Cross-disciplinary fertilisation of mathematical models and methods is very promising but it cannot be mechanistic and must be based on a deep understanding of both similarities and differences associated with different fields of study.

The new trends in application of mathematical methods to social systems of high complexity can be detected in the domain of internet research and advertising, but the exact scope and extent of these applications often remain unknown to the public; algorithms created and tuned to influence human choice are most effective when people are unaware about them. The few cases published in the literature [7,8] point to gathering extensive data on many people, followed by cross-disciplinary analysis and its subsequent application using individually tailored messages. While these examples are often associated with numerous ethical and legal failures, the question of whether these examples have nevertheless introduced any new science or conceptual understanding remains.

Kaiser [7] examined an apparent success in using data collected about voters by the infamous company "Cambridge Analytica" and characterised this approach not only as "effective" but also as "revolutionary". While this approach may indeed have some

intellectual achievements from the practical (although certainly not moral) perspective, does it involve any breakthroughs in science? Experts in public relations know that well-thought and accurately targeted communications are likely to have a more pronounced effect on an individual. The claimed success of Cambridge Analytica had two major factors: (1) delivering personalised messages on a massive scale using modern means of communication and monitoring, and (2) people receiving messages remained unaware that they were placed within a virtual informational environment tailored specifically for them. From the systemic perspective, this is like the spreading of a virus, which is especially fast and effective (for the virus, of course) when we are unaware of its existence. However, after being exposed to various informational infections a few times, people in democratic societies will start learning from their mistakes and acquire some degree of intellectual immunity (and science has an obligation to help). While some people may like personalised messages and services, the second of the two factors listed above is not only unethical but also potentially dangerous for systemic stability.

While this new style of advertising campaigns may involve some intellectual achievements, its apparent successes are more related to the unorthodox breaking of unwritten, ethical and, possibly, legal rules than to principal scientific advances. Determining responses of individuals to personalised advertising does not involve predicting the collective dynamic of propagation of information between different groups of people, which is the essence of complex behaviours in evolutionary systems. The emerging practice of group-orientated messages and services seems to induce polarising trends, which are rather alarming and can become destabilising in democratic societies. The collective dynamic of complex systems needs to be studied, understood, and ultimately conveyed to the public, while the science of modelling complex systems must play a principal role in these advances. In physics, such collective trends correspond to the difference between single-particle and joint multiparticle distribution functions, or between average properties of a single element and complex behaviour of the whole system involving many elements.

In this work, we are more interested in modelling complex systems as a whole rather than in the autonomous modelling of individual elements of these systems. In this context, our goal is to establish fundamental links between modelling approaches used in different domains of science and suitable for complex systems, as well as a broad categorisation of these approaches.

3. Turbulence as the Beginning of Complexity

3.1. Solving Turbulence

In the early 1920s, Arnold Sommerfeld, who was interested in the stability of fluid flows and turbulence, decided to give this problem to his most talented student, Werner Heisenberg. While the student subsequently won the Noble Prize in Physics, the problem of turbulence remains unresolved. It was investigated not only by Heisenberg but also by other most brilliant scientists (Kolmogorov, Batchelor, Obukhov, and many others), who had occasional success, but the full solution of the problem does not seem any closer than it was a century ago. Richard Feynman once reportedly characterised turbulence as "the most important unsolved problem of classical physics". Difficulties with solving the problem of turbulence became commonly known. When, as a junior student, I asked senior fellow students for advice about exciting directions of research, the answer was rather sobering "whatever you do, stay away from turbulence—many tried and all failed". These difficulties that have lasted over a century reflect our first encounter with complexity.

Turbulence is a system of a large dimension that lies at the borders of order and chaos, possessing something we can call a chaotic order. We learned how to describe deterministic mechanical systems and can deal with purely random behaviour (such as that of molecules in thermodynamic objects), but we have difficulties with combinations of both [9]. Turbulence is random and diffusive, and yet it has coherent structures that tend to persist for surprisingly long times. Whatever we can say about turbulence is valid and invalid at the same time. The Kolmogorov theory of inertial interval seems

to be correct [10]. It is correct but it needs refinements to account for fluctuations of the dissipation. These refinements need further refinements to account for intermittency (Kuznetsov and Sabelnikov [11]) and so on. Is Kolmogorov's law of inertial interval correct or incorrect? As in all complex systems, the answer depends on perspective.

While turbulence is a complex system and has similarities with other complex systems, there are noticeable differences between turbulence and what we call complex evolutionary systems—biological, social, economic, and technological systems (most complex adaptive systems are evolutionary of have evolutionary origins). Turbulence does have some inheritance [12] (when large eddies breakup into smaller eddies, the latter inherit some properties of the former), but this inherence is not reliable enough and significant enough to originate any substantial evolutionary processes. Eddies merely keep breaking up until they are dissipated by viscosity. Turbulence is ubiquitous and can be observed at different scales in a lab, in rivers and lakes, in the atmosphere, on other planets, and in the interplanetary space (see Figure 1). It is a mechanical phenomenon, and experiments with turbulence are repeatable, at least on the lab scale. This, however, does not usually apply to complex evolutionary systems; one cannot run one set of economic reforms and then the other one in the same conditions and make an objective comparison. The models developed for turbulence are expected not only to emulate the observed effects but also possess at least some predictive capabilities, while predicting phenomena in complex social systems is often very difficult if not impossible.

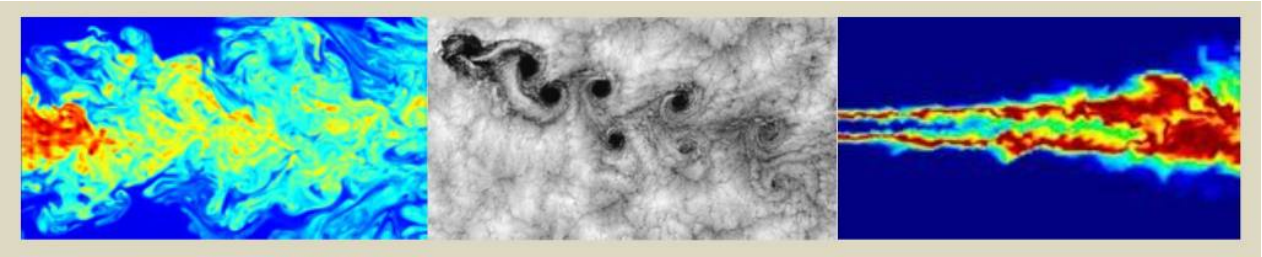

Figure 1. Examples of coherent structure in turbulent flows. Left: experimental laser-induced fluorescence image of a submerged turbulent jet (Fukushima and Westerwee, Wikipedia). Centre: Kármán vortex street induced by wind flowing around the Juan Fernández Islands (NASA, Wikipedia). Right: MMC simulation of Sandia Flame F [13].

Turbulence is essentially the first complex system that science encountered and, therefore, our initial idea of "solving turbulence" in the same way as we solve other mechanical problems was naïve. Complex systems do not have a single ultimate solution; they have many solutions and approaches that should be used under different circumstances. Complex systems permit and, perhaps, demand analyses and modeling using different perspectives. Two seemingly contradictory statements about complex systems may be correct at the same time, depending on qualifications and perspectives.

3.2. Turbulent Reacting Flows

While turbulence is complex, its complexity is to some extent limited. Common models of turbulence are never completely right but neither are they completely wrong in most cases, typically producing a substantial but limited error of 20–40%. The situation changes when we have chemical reactions involved [14]. These reactions are very sensitive, and inaccuracies in modelling can easily give predictions that differ from reality by orders of magnitude [15,16]. Complex evolutionary systems often have complex elements; the elements of human society are humans, which are also complex. Turbulence is a mechanical system, and its elements are notional fluid particles, which are not complex (at least in comparison with humans). The presence of reactions changes this; common combustion of, say, petrol, involves hundreds of species and thousands of chemical reactions which

take place in every fluid particle. Turbulent reacting flows are complex systems comprising complex elements.

Do turbulent reacting flows have evolutionary properties? In the present conditions, these properties do not seem particularly relevant (although one may note that genetic replication can be interpreted as a specific complex form of a chemical reaction). We do not know how the first replicators appeared on Earth, but evolutionary complexity must have emerged from a more basic form of complexity somewhere at the border between order and chaos. The latter provides for variability, while the former allows for some structures to exist, at least for some limited time. It seems that, as the primary and ubiquitous mechanical phenomenon, turbulence in conjunction with chemical reactions could have played a role in creating first replication mechanisms.

3.3. Turbulent Combustion Models

One of the simplest models used in reacting flows is the plug-flow reactor, which assumes an average uniform mixture that gradually evolves from the inlet of the reactor to its outlet [17]. This evolution is specified by the following ordinary differential equations for the average mass fractions:

$$u\frac{d\langle Y_i\rangle}{dx} = W_i(\langle Y_1\rangle, \langle Y_2\rangle, \ldots). \tag{1}$$

This model may work as a reasonable estimate for slow reactions but is rather crude when handling intensive combustion processes.

Another group includes quasi-laminar models that evaluate special variations but neglect turbulent fluctuations. These models are governed by the conventional reactive scalar equations [17].

$$\frac{d\langle Y_i\rangle}{dt} + \mathbf{u}\cdot\nabla\langle Y_i\rangle - \frac{\nabla(D_t\rho\nabla\langle Y_i\rangle)}{\rho} = W_i(\langle Y_1\rangle, \langle Y_2\rangle, \ldots). \tag{2}$$

Using average quantities is inaccurate for most realistic combustion processes. The *plug-flow reactor* and *quasi-laminar* models can be referred to as *average models* or, more precisely, *unconditionally averaged models.*

Conditional models do take into account at least some of the turbulent fluctuations and are reasonably accurate but only for some classes of combustion processes that do not involve more complex phenomena such as extinctions and reignitions. *CMC (conditional moment closure)*, which is the most widely known example of the conditional models is given by the following equations [18]:

$$\frac{dQ_i}{dt} + \langle\mathbf{u}|Z\rangle\cdot\nabla Q_i + \ldots = N_Z\frac{\partial^2 Q_i}{\partial Z^2} + W_i(Q_1, Q_2, \ldots), \tag{3}$$

for $Q_i = \langle Y_i|Z\rangle$, i.e., for the expectation of reactive scalar Y_i, conditioned on a given value of the mixture fraction Z (see Klimenko and Bilger [18] for the complete form of the CMC equation). Here, $N_Z = \left\langle (\nabla Z)^2 \middle| Z \right\rangle$ is the conditional scalar dissipation, $\mathbf{u}$ is velocity, and W is the source term. The models associated with the stationary frame of reference are referred to as *Eulerian*, while models connected to moving fluid are called *Lagrangian*. The conditional and unconditional (quasi-laminar) models specified above are *Eulerian*. The conditional models are intermediate in their complexity and accuracy between quasi-laminar models and Lagrangian PDF models considered below.

The Lagrangian PDF (probability density function) models are used for Monte Carlo simulations of the probability density functions of reactive scalars. These models are formulated using stochastic differential equations.

$$\begin{aligned} &\text{(a) } d\mathbf{x}^{(k)} = \mathbf{u}^{(k)}dt + (2D)^{\frac{1}{2}}d\mathbf{w}^{(k)}(t) \\ &\text{(b) } dY_i^{(k)} = W_i(Y_1, Y_2, \ldots)dt + \widehat{M}\left[Y_i^{(k)}, Y_i^{(m)}, \ldots\right]dt \end{aligned} \tag{4}$$

The superscript k marks different particles, and each of the particles possesses a number of properties $Y_1, Y_2, \ldots$ Here, $\boldsymbol{w}^{(k)}(t)$ denotes the independent Wiener process. The Lagrangian PDF methods were analysed in the seminal work of Pope [19]. The PDF models also allow for *Eulerian* implementations called "stochastic fields" [20]. The synergy of the PDF and conditional methods resulted in the *MMC (multiple mapping conditioning) approach*, which involves adding stochastic equations for the so-called reference variables [21,22],

$$d\xi_l^{(k)} = a_l^{(k)}dt + b_l^{(k)}dw_l^{(k)}(t), \tag{5}$$

to the system in Equation (4) and conditioning [22] of the *mixing operator* $\hat{M}$ [23] not only on physical coordinates $\mathbf{x} = (x_1, x_2, x_3)$ but also on the reference variables $x_1, x_2, \ldots$ MMC models are often implemented combining Eulerian simulations of dynamic properties and sparse Lagrangian simulations of reactive components. Note that using Markov families of larger dimension due to additional (i.e., reference) stochastic variables such as those in Equation (5) allows us to represent a wider spectrum of effects.

In this section, we use notations involving ensemble averages, but the modelling approaches introduced above can also be used in conjunction with *LES (large eddy simulation) filtering* [24]. In LES methods, all fluctuations are divided into resolved fluctuations, which are fully simulated, and sub-filter (sub-grid) scales, which are modelled. Cascade interactions between different scales is an important problem in turbulence. As the filtering scale decreases and approaches the Kolmogorov scales (the scales of the smallest vortices present in a turbulent flow), LES models approach *DNS (direct numerical simulations)*, a complete emulation of the turbulent reacting flows without modelling assumptions.

3.4. Transplantation of Models

As noted above, turbulent combustion has highly sophisticated modelling tools that have been developed over many decades. Quite often, these tools are general and may be used for modelling other complex systems, which are not necessarily directly related to combustion and may range from physical to social systems. Here, we need to distinguish ontological and epistemological sides of this problem. Modelling of complex systems is a less developed but rapidly growing area of scientific enquiry and engineering application.

From the *epistemological* (methodological) perspective, we are interested in modifying and adapting modelling tools and methods to simulate other processes, whether these processes are physically related to combustion or not. The existence of some broad similarities is sufficient.

From the *ontological* (physical) perspective, any complex reality is formed, in one way or another, by numerous chemical kinetic processes that must be consistent with the fundamental laws of thermodynamics. This complex systemic reality is an emergent property of many reactions; it is not reduceable to these reactions but ultimately must be consistent with the fundamental properties of the reaction models.

Despite large differences between different complex systems, we find that these systems tend to have at least some physical similarities, which enables the application of similar modelling methodologies to these systems. In the rest of this article, we try to address the ontological and epistemological sides of the problem examining both methodological and physical implications of using models of varying levels of complexity that are applicable to both combustion systems and general systems.

4. Classes of Systems Models

This section presents major classes of models that can be effectively used for modelling general complex systems introduced by Gell-Mann [25] and many others [26]. If we

account for terminological differences (i.e., agents in fluids simulations are conventionally called particles, whether they represent a physical particle or not), classes of general systems models have their analogues in the different types of models used in simulating turbulent combustion.

4.1. Historical Classification

The most common models used for modelling general systems is *system dynamics* (see Forrester [27]), which involves more conceptual *causal loop diagrams* and more specific *stock and flow diagrams* that help analyse complex systems while dividing them into familiar types of interactions between the elements involved. From the mathematical perspective, the models of system dynamics correspond to a system of ordinary differential equations,

$$\frac{dy_i}{dt} = F_i(\mathbf{y}), \tag{6}$$

which may be both linear and nonlinear. We can easily see that the models of system dynamics (6) use the same class of equations as those used by the plug-flow reactor (1). The models based on ordinary differential equations, such as system dynamics, generally originated in the 1960s and 1970s where typical computer power was sufficient only for solving ODEs. The recent decades have been marked by the emergence of more detailed, yet more computationally expensive models that pertain to partial differential equations, account for motions in physical space, and/or simulate spatially inhomogeneous processes.

While quasi-laminar (2) models can be used in general systems modelling, this is not common. The most comprehensive methods associated with systems modelling are the *agent-based models* [28]. These models involve movements of agents (deterministic and stochastic) and interactions between them. It is easy to see that these models correspond to the PDF models (4) of turbulent combustion, where modelling agents are represented by notional particles. For general systems modelling, the mixing operator M needs to be generalised to reflect various possible types of interactions between agents (particles). Interactions of elements in evolutionary systems are often *competitive*. It would be reasonable to call more general versions of *M* the "*interaction operator*" [4,12]. These generalisations are considered in the next section. A class of models called *cellular automata* [28] can be seen as a special case of agent-based models where agents interact with their neighbours without moving in physical space. Cellular automata usually presume relatively simple interaction algorithms, illustrating a principle rather than modelling realistic physical objects. Overall, cellular automata are more historical than the conceptual category; models called agent-based can also have non-moving agents.

While conditional and LES-type models are well developed for (and extensively used in) combustion modelling, application of these approaches to general systems seems quite promising but uncommon at present. Lastly, we note that comprehensive DNS-type modelling resolving the smallest details of the processes under consideration is very difficult for turbulent combustion but practically impossible for complex systems due to their complex, multidimensional, multiscale, and hierarchal nature. The correspondence of turbulent combustion and general system models is summarised in Table 1.

Table 1. Relations between turbulent combustion and general system models.

Models for Turbulent Reacting Flows	Models for General Complex Systems
Average and quasi-laminar models, plug-flow reactor	System dynamics and other models dealing with direct emulation of overall performance of the system
PDF Monte Carlo models, Largangian particle implementations, mixing	Agent-based models with interaction between moving agents; particles are called agents
Eulerian implementation of stochastic simulations (e.g., stochastic fields)	Stationary agents and/or cellular automata, where agents do not move and usually represented by stationary cells

Table 1. *Cont.*

Models for Turbulent Reacting Flows	Models for General Complex Systems
Conditional models and conditional/PDF models	Elements of conditional methods are used occasionally but the methodology is not well developed for general systems
LES and similar models with direct simulation of large scales and modelling small scales	Reproducing large scales in conjunctions with a simplified treatment of processes at small-scales is promising, especially in conjunction with conditional models
DNS or complete simulation of all (from large-scale to small-scale) features	Modelling of all details is usually impossible for general complex systems

4.2. Conceptual Classification

First, we must distinguish average models that simulate the overall properties of complex systems and agent-based models that reproduce properties of complex systems by emulating behaviours of multiple elements. System dynamics is, perhaps, the best-known approach to average modelling, but the average category can involve many other methods. For example, the behaviour of complex systems may be reproduced by using neural networks or other forms of AI [20].

Among the agent-based models, we distinguish global, Eulerian, Lagrangian, and combined models. In global models, agents interact globally without any constraints imposed by localisation. This can simulate homogeneous conditions (e.g., homogeneous turbulence) or correspond to instantaneous interactions at long distances. The other types of models (i.e., Eulerian and Lagrangian) involve localisation in physical space (or any other localisation space, for example, using the mixture fraction space in MMC), where agents interact only with their neighbours. In Eulerian models, the agents are stationary, for example, representing nodes, cells, or locations, as in cellular automata models. In Lagrangian models, the agents (or particles, as agents are called in fluids applications) move and, consequently, interact with different neighbours. The motion can involve both directional and random components.

Lastly, global, Eulerian, and Lagrangian models can be combined. For example, propagation of information within a population involves a network of stationary, Eulerian agents (individuals or groups of individuals), and each of these agents possesses a set of properties characterising human behaviour, while information is represented by Lagrangian agents, which move between Eulerian nodes and possess a different set of properties. In the context of modelling reaction flows, MMC, which was mentioned in Section 3.3, combines Eulerian and Lagrangian characteristics into a single model.

The major classes of models used in simulating complex systems can be summarised as follows:

- **Average models**
  - System dynamics
  - Other average models (AI, neural networks, . . .)
- **Agent-based models (Monte Carlo and particle methods)**
  - Global (homogeneous)
  - Eulerian
  - Lagrangian
  - Combined (Eulerian–Lagrangian)
- **Modified and hybrid models**
  - Conditional, multiscale, multilevel, etc.

The group of modified and hybrid models is added to the classification to account for various modifications and combinations of the models. Conditional models either involve some kind of incomplete (conditional) averages or, as applied in MMC, enforce some conditional properties on the behaviour of the agents. Different models can be used at

different scales and different levels of systemic hierarchy. Elements of a complex system are often complex systems on their own. These elements can be represented by agents, and each of these agents is linked to another model associated with the complex behaviour of the subsystems. Each of these subsystems can have elements that are also complex systems. In addition, we may distinguish, as conventionally applied in turbulence, macroscopic and microscopic processes.

While possibilities of combining different models in simulating complex systems are limitless, we need to raise a voice of caution. Complex systems are usually far too complex for modelling everything down to the smallest details as achieved in DNS. Practical success can be achieved by modelling certain features of interest associated with a complex system. A reasonable traffic model does not need to involve modelling mood for each driver. If a complex system consists of elements represented by complex subsystems, we face two types of complexity: (1) the emergent complexity associated with collective actions of elements, and (2) the complexity inherited from each element. While modelling a complex system, we are (and should be) predominately concerned with the emergent complexity, since this is the central element of systemic analysis, allowing us to achieve a practical outcome with a reasonable investment of resources. The complexities associated with each element often partially negate each other to form common statistical properties. In physics, for example, statistical thermodynamic properties often become independent of the detailed characteristics of the elements (molecules). While full-scale multilevel modelling can be avoided in many cases, this avoidance cannot be always guaranteed, and model hybridisation may become a necessity.

5. Major Features of Complex Systems and Models

This section outlines conceptual similarities and major differences that need to be bridged between combustion and systems modelling. In this context, a number of features need to be considered from both ontological and epistemological perspectives.

5.1. Modelling Multiscale Processes

Turbulent combustion processes have a wide range of scales, typically from 10^{-5} to 10^{-1} s for turbulence and from 10^{-9} to 1 s for chemical kinetics [17]. Interactions of different scales are one of the major problems that turbulent combustion models need to deal with. For example, the Flamelet model [11,29] is very effective in dealing with fast localised reactions interacting with slower and larger turbulence, while MMC implements PDF treatment of smaller scales combined with conditional modelling at larger scales [22].

While complex systems usually involve multiscale interactions of systemic hierarchies, multiscale modelling is less common due to a dramatic increase in complexity. Modelling strategies for complex systems usually involve significant simplifications focusing on a particular time scale and on a particular level in the hierarchy of emergent systems. The range of nine orders of magnitude would correspond to the range of scales between 1 h and 1 M years. While modelling such a range is neither practical nor feasible, studying interactions between more close and more related scales is to become common in the future.

Complex systems are hierarchal when, for example, elements of a system are also systems consisting of more minute elements. Multiscale and multilevel properties of complex systems are usually closely related to each other. Modelling multilevel hierarchal systems can be difficult and often requires simplifications.

5.2. Conserved Properties and Information

Speaking about properties of systems and their elements, we need to distinguish conservative properties, which are preserved (or changed due to transport, sinks, and sources), and information, which is not preserved and can be easily replicated or destroyed. The stock and flow diagrams of system dynamics [30] distinguish stocks that change due to flows and feedback loop information that can be easily multiplied or divided by a constant.

The quantities used in chemical kinetics are conservative and are either preserved (e.g., energy and elements) or changed only due to reactions. The conventional mixing operator M is, therefore, conservative. While it can be easily generalised to handle information (for example, competitive mixing considered by Klimenko and Pope [4]), this addresses the problem epistemically but not ontologically. The emergence of information from conservative properties is a principal step that needs explanation; information used by biological and social systems must be based upon some chemical or physical transformations. It appears, however, that information emerges even in conventional reacting flows, specifically in premixed combustion.

In turbulent premixed combustion (whose accurate modelling remains one the most difficult unresolved problems of the 20th century), the two major states (fresh and burned) are separated by a very thin transitional region, which we can overlook for this discussion. A fluid particle in the fresh state y_f transits to the burned state y_b when and only when it receives a temperature boost from another burned particle [4].

$$\begin{array}{l} y_f^{(k)} + y_f^{(l)} \to y_f^{(k)} + y_f^{(l)} \\ y_f^{(k)} + y_b^{(l)} \to y_b^{(k)} + y_b^{(l)} \\ y_b^{(k)} + y_b^{(l)} \to y_b^{(k)} + y_b^{(l)} \end{array} \tag{7}$$

where we can assume that $y_f = 0$ and $y_b = 1$; in combustion, such a variable y is conventionally called the reaction progress variable. The possibility of extinction is not considered in this model. If we have many particles in a uniform container, then

$$\frac{d\langle y \rangle}{dt} = W = c\langle y \rangle (1 - \langle y \rangle), \tag{8}$$

where $<y>$ and $1 - <y>$ specify the average fractions of the burned and fresh particles, and the constant c is proportional to the probability of interaction between two particles. Equation (8) corresponds to the BML (Bray–Moss–Libby) model of turbulent premixed combustion and at the same time; this is the so-called logistic equation—a model for the propagation of innovation or simulation of a simple epidemic [4]. It is easy to see that (8) can be integrated $<y> = (1 + e^{-ct})^{-1}$.

It is obvious that transformation (7) replicates 1 bit of information from particle "*l*" to particle "*k*", which underpins the wide systemic applicability of the logistic equation given by (8). Therefore, while chemical kinetics deals with conserved properties, it can emulate replication of information—the principal element of all complex evolutionary systems—even under conditions of common combustion processes. The distinction of conserved properties, information, and signals is blurred.

5.3. Emergence of Chaotic Order

One of the most principal assumptions known in modern physics is the hypothesis of molecular chaos of Ludwig Boltzmann. The main implication of this hypothesis is Boltzmann's H-theorem that aligns kinetic equations with the second law of thermodynamics. Considering systems of notional particles or agents [31,32], the hypothesis of chaos can be expressed by $P(\mathbf{y}^{(k)}, \mathbf{y}^{(l)}) = P(\mathbf{y}^{(k)})P(\mathbf{y}^{(l)})$, where $P(\mathbf{y}^{(k)})$ is probability of particle k having properties $\mathbf{y}^{(k)}$. This hypothesis imposes severe constraints on the complexity of the system, restricting system behaviour to basic thermodynamics-like randomness and prohibiting hierarchal multiscale dependencies. Further research into the particle systems indicates that dependencies violating particle chaos emerge under some conditions [31]. This generally is not desirable in conventional combustion simulations but can be instrumental in simulating complex systemic effects.

5.4. Emergence of Intransitivity

Chemical kinetics is always compliant with the laws of thermodynamics, which enforces transitive total preorder of the states of the system as determined by increasing entropy (or decreasing Gibbs free energy—Gyftopoulos and

Beretta [33]). Therefore, kinetic systems usually relax towards equilibrium or partial equilibrium without oscillations. This is in contrast with many complex systems where cyclic behaviours are quite common [12,34].

We need to note that thermodynamic constraints mentioned above are unbreachable only for closed systems. External interference can, at least in principle, reduce systemic entropy. Yet, oscillations are not common for chemical reactions, even in open systems. In this context, the example of periodic evolution (in open systems, of course) of the Belousov–Zhabotinsky reaction [35] clearly indicates that neither thermodynamics nor reaction kinetics prohibits cyclic behaviour. While transitive competitions can be accounted for by effective thermodynamics [12], the emergence of intransitivity [34,36] is an important step in developing the complexity of evolutionary systems [37]. Intransitivity should be expected to emerge naturally in open systems.

5.5. Complex Topologies, Networks and Emergence of the Small World

The models we primarily consider above are formulated either for homogeneous conditions or for plain physical space. Numerical methods use uniform rectangular grids to represent the topology of plain spaces. Modern models, however, may need to deal with more complex topological connectivity. For reacting flows in porous media, this connectivity can be expressed by a complex network of pores of different sizes [38]. The models developed for turbulent combustion [39] can also be useful for evaluation of reactive transport in porous medium; however, in the case of particle-based models, they need to replace random walk in the open physical space with random walk on graphs that reflect the structure of the porous medium [40,41].

A general expression for Markov random walk on graphs is given by the following recurrent expression:

$$\mathbf{p}^{(n+1)} = \mathbf{T}\cdot\mathbf{p}^{(n)}, \tag{9}$$

for probabilities $\mathbf{p}^{(n)} = (p_1, p_2, \ldots, p_k)^{(n)}$ of particle location at nodes 1, 2, … , k for the timestep n. Here, $\mathbf{T}$ is the stochastic matrix (positive elements summing up to unity for each column), which specifies Markov transition probabilities [41].

For complex general systems, network structure appears to be even more important [40]. In such networks, localised links between nodes may be combined with long-distance connections. For example, using models (7)–(8) for simulation of a simple epidemic may need to take into account not only local travel, which may be approximated by a conventional Brownian-type random walk (such as Equation (4a)), as well as occasional long-distance flights. Considering the representation of connectivity by a graph, these flights correspond to occasional connections between remote nodes. For such graphs, we face a new phenomenon called the small-world effect when the number of nodes n_r in a graph grows exponentially $n_r \sim \exp(cr)$ with the distance r from a selected central node [42]. This is in contrast with $n_r \sim r^2$ for a localised grid on a two-dimensional surface. This small-world effect results in an exponentially fast propagation of epidemic, making the modern interconnected world more capable of and more susceptible to the fast propagation of information and viruses.

6. Concluding Remarks

Modelling reacting flows has been developed over many decades offering a spectrum of modelling methodologies with a wide range of complexity and refinement. The success of this development is largely determined by the availability of experimental data and the repeatability of experiments. While turbulence and realistic combustion kinetics are complex

systems, modelling tools in combustion can always be checked against experiments or more detailed simulations.

Over many decades, studies of complex evolutionary systems could not enjoy the same level of verifiability and quantification and often had to resort to more qualitative analysis and observation. While reacting flows commonly allow for a definite formulation of the problem, this is usually not the case with complex socioeconomic systems, where even formulation of the problem is subject to a substantial degree of ambiguity, and proper experimental validation is often impossible. It is not a surprise that modelling of general complex systems was limited to more basic (yet still very useful, of course) approaches, such as system dynamics.

The age of the internet brought new conditions of effective communication networks and availability of social data, which will have far-reaching implications for further technological development and social dynamic. Some of these implications are undoubtedly positive and some are not. The availability of data opens possibilities for the quantification of social science and expansion of applications and methods previously used only in physics and mathematics to a much wider spectrum of problems. More effective and experiment-tested types of models can be applied to various complex evolutionary systems addressing numerous social and environmental challenges that humankind has to face [43]. These opportunities, however, are often forfeited in favour of ad hoc applications of available data to achieve immediate political and economic gains. While it is not raw data but the ability to construct a suitable model or theoretical framework using these data that can be successful, publicly available information indicate noticeable intensification in using data for political and economic gains. This intensification, however, does not extend to the main issue associated with complex evolutionary systems—the patterns of collective emergent behaviours.

Without introducing any new models, we demonstrate a broad consistency of models for reacting flows and general complex systems and examine two types of issues: physical (ontological) and methodological (epistemological). It is arguable that, while having numerous emergent properties, complex systems involve, at some basic level, transport and reaction; therefore, they must be consistent with the laws controlling reacting flows. Here, we discuss that reacting systems do allow for the emergence of multiscale behaviour, information, chaotic order, and cyclic intransitivity. Previously, we demonstrated the emergence of cooperation in general intransitive systems with intransitive competition. Note that a reduction of complex behaviour to the level of chemical reactions is usually either impossible or impractical and certainly is not proposed or advocated here.

Hence, further progress in modern methodologies for modelling complex systems (which involve not only physical but also social, economic, and technological processes) is likely to implement, explicitly or implicitly, the extensive set of methods developed in combustion modelling in conjunction with necessary adjustments and adaptations of these models to more general environments.

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References

1. Mayer-Schonberger, V.; Cukier, K. *Big Data: A Revolution that Will Transform How We Live, Work, and Think*; Mariner Books: Boston, MA, USA, 2014.
2. Pope, S.B. *Turbulent Flows*; Cambridge University Press: Cambridge, UK, 2000.
3. Klimenko, A.Y. The convergence of combustion models and compliance with the Kolmogorov scaling of turbulence. *Phys. Fluids* **2021**, *33*, 25112. [CrossRef]

4. Klimenko, A.Y.; Pope, S.B. Propagation speed of combustion and invasion waves in stochastic simulations with competitive mixing. *Combust. Theory Model.* **2012**, *16*, 679–714. [CrossRef]
5. Bryant, A. Liquid modernity, complexity and turbulence. *Theory Cult. Soc.* **2007**, *24*, 127–135. [CrossRef]
6. Eisenhauer, W.I. Big problems with big data. *ISE Ind. Syst. Eng. Work* **2016**, *48*, 22.
7. Kaiser, B. *Targeted*; HarperCollins Publishers: New York, NY, USA, 2019.
8. Cummings, D. The Campaign, Physics and Data Science. 2016. Available online: https://dominiccummings.com/2016/10/29/on-the-referendum-20-the-campaign-physics-and-data-science-vote-leaves-voter-intention-collection-system-vics-now-available-for-all/ (accessed on 17 May 2022).
9. Heinz, S. *Statistical Mechanics of Turbulent Flows*; Springer: Berlin/Heidelberg, Germany, 2003.
10. Frisch, U. *Turbulence: The legacy of A.N. Kolmogorov*; Cambridge University Press: Cambridge, UK, 1995.
11. Kuznetsov, V.R.; Sabelnikov, V.A. *Turbulence and Combustion*, 2nd ed.; Hemisphere: New York, NY, USA, 1990.
12. Klimenko, A.Y. Complex competitive systems and competitive thermodynamics. *Phil. Trans. R. Soc. A* **2013**, *371*, 20120244. [CrossRef]
13. Ge, Y.; Cleary, M.J.; Klimenko, A.Y. A comparative study of sandia flame series (d–f) using sparse-lagrangian mmc modelling. *Proc. Combust. Inst.* **2013**, *34*, 1325–1332. [CrossRef]
14. Williams, F.A. *Combustion Theory*, 2nd ed.; Addison-Wesley, Reading: Boston, MA, USA, 1985.
15. Libby, P.A.; Williams, F.A. *Turbulent Reactive Flows*; Springer: Berlin/Heidelberg, Germany, 1980.
16. Fox, R. *Computational Models for Turbulent Reacting Flows*; Cambridge University Press: Cambridge, UK, 2003.
17. Warnatz, J.; Maas, U.; Dibble, R.W. *Combustion: Physical and Chemical Fundamentals, Modelling and Simulation, Experiments, Pollutant Formation*; Springer: Berlin/Heidelberg, Germany, 1996.
18. Klimenko, A.Y.; Bilger, R.W. Conditional moment closure for turbulent combustion. *Prog. Moment Energy Combust. Sci.* **1999**, *25*, 595–687. [CrossRef]
19. Pope, S.B. Pdf methods for turbulent reactive flows. *Prog. Energy Combust. Sci.* **1985**, *11*, 119–192. [CrossRef]
20. Readshaw, T.; Ding, T.; Rigopoulos, S.; Jones, W.P. Modeling of turbulent flames with the large eddy simulation; probability density function (pdf) approach, stochastic fields, and artificial neural networks. *Phys. Fluids* **2021**, *33*, 035154. [CrossRef]
21. Klimenko, A.Y.; Pope, S.B. A model for turbulent reactive flows based on multiple mapping conditioning. *Phys. Fluids* **2003**, *15*, 1907–1925. [CrossRef]
22. Sundaram, B.; Klimenko, A.Y.; Cleary, M.J.; Ge, Y. A direct approach to generalised multiple mapping conditioning for selected turbulent diffusion flame cases. *Combust. Theory Model.* **2016**, *20*, 735–764. [CrossRef]
23. Sawford, B. Micro-mixing modelling of scalar fluctuations for plumes in homogeneous turbulence. *Flow Turbul. Combust.* **2004**, *72*, 133–160. [CrossRef]
24. Rogallo, R.S.; Moin, P. Ten questions concerning the large-eddy simulation of turbulent flows. *Annu. Rev. Fluid Mech.* **1984**, *16*, 99–137. [CrossRef]
25. Gell-Mann, M. *The Quark and the Jaguar*; W.H. Freemen and Company: New York, NY, USA, 1994.
26. Gilbert, G.N.; Troitzsch, K.G. *Simulation for the Social Scientist*, 2nd ed.; Open University Press: Maidenhead, UK, 2005.
27. Forrester, J.W. System dynamics-the next fifty years. *Syst. Dyn. Rev.* **2007**, *23*, 359–370. [CrossRef]
28. Clarke, K.C. *Cellular Automata and Agent-Based Models*; Springer: Berlin/Heidelberg, Germany, 2014; pp. 1217–1233.
29. Peters, N. *Turbulent Combustion*; Cambridge University Press: Cambridge, UK, 2000.
30. Sterman, J.D. *Business Dynamics: Systems Thinking and Modeling for a Complex World*; Irwin/McGraw-Hill: Boston, MA, USA, 2000.
31. Klimenko, A.Y. Lagrangian particles with mixing. I. simulating scalar transport. *Phys. Fluids* **2009**, *21*, 065101. [CrossRef]
32. Klimenko, A.Y. Lagrangian particles with mixing. II. sparse-lagrangian methods in application for turbulent reacting flows. *Phys. Fluids* **2009**, *21*, 065102. [CrossRef]
33. Gyftopoulos, E.P.; Beretta, G.P. *Thermodynamics. Foundations and Applications*; Macmillan: New York, NY, USA, 1991.
34. Klimenko, A.Y. Complexity and intransitivity in technological development. *J. Syst. Sci. Syst. Eng.* **2014**, *23*, 128–152. [CrossRef]
35. Zhabotinsky, A. Belousov-Zhabotinsky reaction. *Scholarpedia* **2007**, *2*, 1435. [CrossRef]
36. Poddiakov, A.; Valsiner, J. Intransitivity cycles and their transformations: How dynamically adapting systems function. In *Qualitative Mathematics for the Social Sciences: Mathematical Models for Research on Cultural Dynamics*; Rudolph, L., Ed.; Routledge Abingdon: New York, NY, USA, 2013; pp. 343–391.
37. Klimenko, A.Y.; Klimenko, D.A. *The Evolution of Technology and Emergence of the Knowledge Society*; Glasstree Academic Publishing: Morrisville, NC, USA, 2019.
38. Klimenko, A.Y.; Saulov, D.N.; Massarotto, P.; Rudolph, V. Conditional model for sorption in porous media with fractal properties. *Transp. Porous Media* **2012**, *92*, 745–765. [CrossRef]
39. Klimenko, A.Y.; Abdel-Jawad, M.M. Conditional methods for continuum reacting flows in porous media. *Proc. Combust. Inst.* **2007**, *31*, 2107–2115. [CrossRef]
40. Klimenko, D.A.; Hooman, K.; Klimenko, A.Y. Evaluating transport in irregular pore networks. *Phys. Rev. E* **2012**, *86*, 011112. [CrossRef] [PubMed]
41. Bouet, V.; Klimenko, A.Y. Graph clustering in industrial networks. *IMA J. Appl. Math.* **2019**, *84*, 1177–1202. [CrossRef]

42. O'Sullivan, D. *Spatial Network Analysis*; Springer: Berlin/Heidelberg, Germany, 2014; pp. 1252–1273.
43. Mensah, P.; Katerere, D.; Hachigonta, S.; Roodt, A. *Systems Analysis Approach for Complex Global Challenges*; Springer: Cham, Switzerland, 2018.