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Letter

Machine learning for modeling, diagnostics, and control of non-equilibrium plasmas

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Abstract

Machine learning (ML) is a set of computational tools that can analyze and utilize large amounts of data for many different purposes. Recent breakthroughs in ML and artificial intelligence largely enabled by advances in computing power and parallel computing present cross-disciplinary research opportunities to exploit some of these techniques in the field of non-equilibrium plasma (NEP) studies. This paper presents our perspectives on how ML can potentially transform modeling and simulation, real-time monitoring, and control of NEP.

Keywords: non-equilibrium plasma, machine learning, artificial intelligence

(Some figures may appear in colour only in the online journal)

Machine learning (ML) is a branch of artificial intelligence that seeks to find patterns from statistical or probabilistic analysis of large amounts of data [1]. The data that can be used for ML can take many different forms—so-called heterogeneous and unstructured datasets. Recent advances in computing power and parallel computing such as graphics processing unit architectures or cloud-based computing platforms, as well as advances in automated data acquisition capabilities, have facilitated widespread adoption of ML for development of complex models that can process and learn from large sets of unstructured data.

The fundamental idea in ML is that, for many applications, training a computer algorithm for predicting or finding patterns in the behavior of a complex system by observing many input–output samples of its behavior can be significantly simpler than programming a set of rules (e.g. developing physics-based models) [2]. Many of the ideas underlying this data-driven approach to modeling complex systems have been known for years, but only recently has it become practical to obtain and analyze the enormous quantities of data needed for the schemes to work. This paper aims to present our perspectives on how ML can potentially transform modeling and simulation, diagnostics, and control of non-equilibrium plasma (NEP). We first describe key distinctions in the various types of ML methods, and then provide an overview of the type of research questions in modeling and operation of NEP for which ML can be appropriate. The emerging ML-based tools for modeling, diagnosis, and control appear to be especially promising for atmospheric pressure plasmas applied to complex systems such as complex surfaces or even to biological systems.

Machine learning

ML methods can be broadly categorized into three main paradigms: supervised, unsupervised, and reinforcement learning [2]. If the machine is given output data that is to be matched with input data, the learning is said to be *supervised* [3]. Supervised learning methods utilize so-called *labeled* training data consisting of many examples of input and output results. The machine then is able to make predictions about *unlabeled* examples. The nature of the output (i.e. the label) can take various forms, including discrete components in classification methods, real-valued components in regression methods, or a mixture of discrete and real-valued components. In plasma applications, output can range from chemical, physical, and electrical properties of a target surface [4–6] to plasma properties such as degrees of molecular gas dissociation, plasma density, electron energy, neutral species rotational and vibrational temperature [6], or energetic and angular distribution of sputtered particles [7]. Input features for these ML applications in a plasma context can include, for example, optical emission spectra, current–voltage signals, electro-acoustic emission measurements, laser-induced fluorescence data, mass spectrometry data, and visual imaging. In other words, any measured information about the state of the plasma can be utilized as *input data* to predict various properties of the plasma or its effects on adjacent surfaces as *output data*.

Supervised learning systems generally aim to learn a *mapping* between the inputs and outputs via determining the 'optimal' combination of input features that minimizes the difference between the predicted and actual outputs. There exists a variety of forms of input–output mapping, including decision trees, decision forests, logistic regression, support vector machines, kernel machines, neural networks, and Bayesian classifiers, where algorithms for learning the mapping from data often rely on optimization or numerical analysis [3, 8]. *Deep learning* has been an important area of progress in supervised learning in recent years. Deep learning systems consist of multilayer networks of nonlinear processing units, where each network layer computes learned representations of the input features [9]. Modern parallel computing architectures have enabled the construction of deep learning systems with billions of processing units that can be trained on very large collections of data. These approaches have proven extraordinarily successful, for example, in computer vision and speech recognition applications.

Unsupervised learning, on the other hand, involves the analysis of unlabeled data under assumptions about structural properties of the data [3, 8]. Unsupervised learning is particularly useful for finding hidden structures or relationships within unlabeled data. As a common application of unsupervised learning, *clustering* aims at determining a partition of the data (and possibly a rule for partitioning future data) in the absence of explicit labels for a desired partition. Another application is *dimension reduction* methods such as principal component analysis that make specific assumptions about a low-dimensional manifold that data lie on, and aim to identify that manifold explicitly from data [3]. Unsupervised learning, for example, can be used for discovering patterns in characteristics of a target surface in plasma–surface applications [6], or extracting latent information from plasma diagnostics [10]. Unsupervised learning can also be applied as a preparatory step in identifying key features and assigning labels for subsequent supervised learning.

Reinforcement learning is another major ML paradigm, where the information of the training data is intermediate between supervised and unsupervised learning [11, 12]. The training data in reinforcement learning provide only an indication as to whether an action is correct or not, rather than containing the correct output for a given input. Generally, the learning task in reinforcement learning is to determine actions for an agent acting in an unknown dynamical environment such that the learned actions maximize the expected reward of the agent over time. Thus, reinforcement learning systems aim to determine the 'ideal' behavior of an agent within a specific context based on feedback from the agent's response. As such, reinforcement learning algorithms commonly rely on ideas and methods from optimal control theory and operations research. Robotic- assisted operation of NEP, for example, in treatment of complex surfaces or surgical procedures is a promising future application of reinforcement learning.

Although the three ML paradigms help organize the most commonly used learning methods, current developments also involve blends across these paradigms [2]. Among the main considerations in selecting the appropriate ML method for a given application are the sample complexity (i.e. the amount of data that is required to learn accurately), the computational complexity (i.e. the required computational resources), and the representation (i.e. mathematical structures) that the learning algorithm uses for what it learns. The diversity of the ML methods reflects the diverse requirements of applications, which depend on varying trade-offs between sample complexity, computational complexity, and performance.

Machine learning for modeling and simulation of NEP

Much effort has been invested in the high-fidelity modeling and simulation of the behavior of NEPs to obtain better understanding of the basic physical and chemical mechanisms of interactions between the plasma and complex surfaces. ML can aid in the development of predictive models for NEPs in two primary ways: (i) learning computationally efficient *surrogate models* for physics-based predictive models, and (ii) learning models for plasma-surface interactions and plasma-induced surface effects from experiments when there is a lack of comprehensive theoretical models for the fundamental plasma-surface interaction mechanisms.

There is a variety of models and simulation strategies for NEPs, such as fluid, particle, or hybrid fluid-particle models. These models can predict the spatio-tempo distributions of the charged particle densities and energies, the self-consistent electric field and currents, neutral species densities and temperature, species fluxes internally and at surfaces [13–16]. However, these physics-based modeling approaches are generally computationally expensive and in many cases may not be amenable to extensive and repeated computer simulations. The computational complexity of plasma simulations can further increase when incorporating surface effects of the plasma that may occur across multiple length- and time-scales [17]. Supervised learning methods such as artificial neural networks, support vector machines, and kriging models can be used to develop surrogate models that are compact and significantly cheaper to evaluate than the high-fidelity predictive models [18]. Surrogate models (also known as metamodels, or response surface models) are constructed using simulation data from high-fidelity models, and are essentially approximate models that provide black-box relationships between inputs and outputs of a system. Surrogate modeling has proven useful in various fields of science and engineering (e.g. computational biology and chemistry [19, 20]) for tasks such as design of experiments and design space visualization, sensitivity analysis, parameter estimation, and optimization. In modeling and simulation of NEPs, the notion of surrogate modeling can be used for deriving approximate plasma-surface interface models that bridge the different length- and time-scales of the fundamental plasma and surface processes. This approach may prove useful especially in simulation of NEP processes that involve formation of micro- and nano-structured materials at surfaces, where plasma simulations that span length scales on the order of 1 m can pose a significant computational challenge. Hence, surrogate modeling offers the ability to develop multiscale models for complex plasma-surface interactions that are significantly more efficient than combined theoretical models of the plasma and surface processes. For example, artificial neural networks trained using theoretical simulations are shown to be useful for modeling the interactions of energetic particles with a surface and the subsequent particle transport in thin film formation via plasma sputtering [7]; see figure 1. Nonetheless, the main challenge in surrogate modeling is how to obtain an approximate model from the simulation data that is as accurate as possible over some domain of interest while minimizing the simulation cost of the data generation. This challenge necessitates the appropriate selection of the structure and complexity of the surrogate model, the number and distribution of the simulation data used for learning the surrogate model, and the validation methods used for estimating the quality of the model [21].

Machine learning also holds great promise for data-driven modeling of NEPs. The term *data-driven modeling* commonly refers to building models from experimental data, as opposed to physics-based models. Data-driven models are essentially 'black-box' models that exploit an enormous collection of measurements connecting input and output data. In particular, supervised learning may prove useful for modeling plasma interactions with complex surfaces as well as the resulting plasma-induced surface effects. Plasma–surface mechanisms are generally among the least-understood aspects of NEPs interacting with complex surfaces. The induced surface effects depend on a multitude of factors, including the plasma chemistry, the nature of the surface, and the operating parameters of the NEP. The relationship between such factors and the plasma-induced surface effects can have complex and nonlinear character. Supervised learning offers the ability to learn nonlinear, multidimensional functional relationships directly from input–output data, without prior assumptions about the nature of the relationships. In fact, there is a relatively large body of literature on the use of artificial neural networks for constructing nonlinear models for various plasma-based processes such as plasma etch [23, 24], plasma-enhanced chemical vapor deposition [25], plasma-induced surface modification [5], and atmospheric plasma spray processes [4, 22, 26]. These nonlinear models, which are constructed from experimental data and can be static or dynamic, commonly describe the effect of multiple process input parameters (e.g. flow rates of input gases, pressure, power, frequency, electrode spacing) and/or surface properties (e.g. electrical or chemical characteristics of the surface) on the plasma-induced process outputs (e.g. etch rate and selectivity in plasma etch, coating characteristics in surface modification, or in-flight particle characteristics in atmospheric plasma spray); see, e.g. figure 2. Such predictive models provide useful *forward* mappings between the process inputs and outputs to systematically elucidate the effects of various plasma parameters and/or surface characteristics on the plasma-surface interactions. Alternatively, supervised-learning models can be used to learn the *inverse* relationship of the process. Inverse relationships can greatly facilitate systematic exploration of the process design space and design of experiments, especially for NEP processes such as plasma etch that have an enormous process parameter space. Yet, a main challenge in learning these types of models can arise from the large number of process parameters and the interdependencies between them, particularly in the light of limited availability of experimental data for training a model. Unsupervised learning methods for dimension reduction are useful for input feature selection. Removing irrelevant and noisy features will enable building simpler and more accurate models that generalize better to unseen data.

Leveraging the separation of time-scales of the plasma and surface processes, plasma–surface interface models learned from experiments can also be combined with physics-based models of NEPs. The resulting multiscale models would allow predicting the complex effects of the 'plasma outputs' (e.g. reactive/excited species fluxes, charging, electric field emission, photon fluxes, or localized heating) on the surface response. As such, supervised learning of plasma-surface interface models can help elucidate fundamental surface mechanisms, for example, in plasma catalysis [27] or plasma medicine [28] where mechanistic understanding of the complex surface effects of NEP is generally limited. On the other hand, recent advances in the use of ML and deep learning for predicting radiation therapy outcomes in radiation oncology can guide the development of appropriate ML tools for modeling and quantification of *plasma dose* in plasma medicine [29–31]. Plasma dose modeling is an important step toward personalization of plasma dose prescription and control of a patient's response in plasma medicine. Some of the main input features that can be incorporated into a plasma dose model for predicting the treatment outcome include clinical features such as patient information, treatment features such as the spatio-tempo distribution of the chemical, physical, and electrical effects of the plasma delivered to the target, molecular features such as those pertaining to the cellular biochemistry in the target, and imaging features such as size and volume of the target.

Machine learning for diagnostics of NEP

Direct and quantitative diagnosis of NEPs generally poses a significant challenge. Quantitative diagnostic techniques such as laser-induced fluorescence, mass spectrometry, or spontaneous Raman scattering commonly require sophisticated instrumentation and specialized experimental configurations that can restrict the operational flexibility of NEPs [33–35]. On the other hand, relatively inexpensive, simple, and easy-to-implement NEP diagnostics such as optical and electro-acoustic emission spectroscopy can contain a wealth

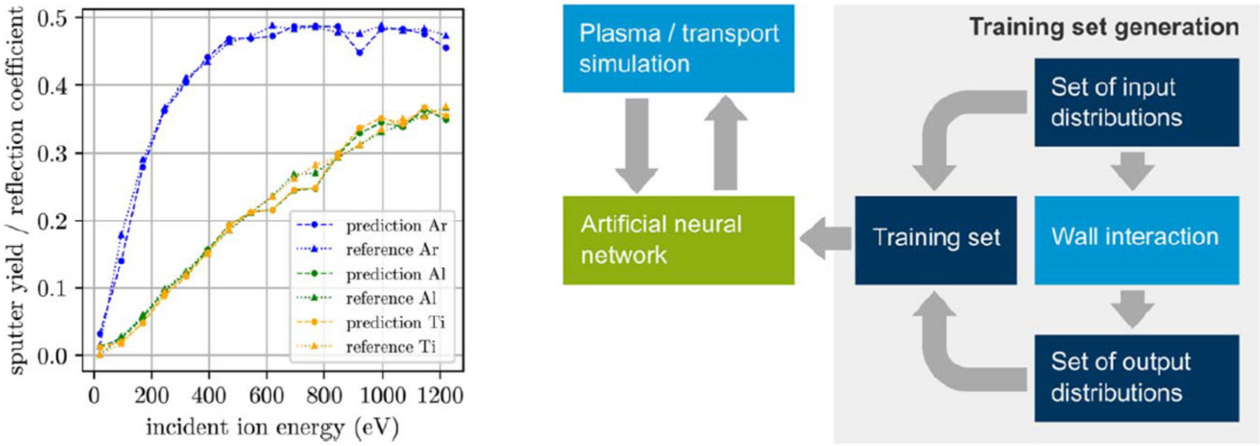

Figure 1. Supervised learning enables construction of computationally efficient surrogate models from theoretical simulation data for multiscale modeling of plasma-surface interactions across multiple length- and time-scales. Here, artificial neural networks were used to develop a plasma–surface interface model for a plasma sputtering process. The interface model was used for predicting the energetic and angular distribution of surface species ejected into the plasma as a function of energy distributions of incident species. Accordingly, the interface model allowed for predicting the inflow of particles in the gas-phase model. The plot on the left depicts the predicted sputter yield (Al/Ti) and reflection coefficient (Ar) by the artificial neural network as a function of incident projectile energy. Reproduced from [7]. © IOP Publishing Ltd. All rights reserved.

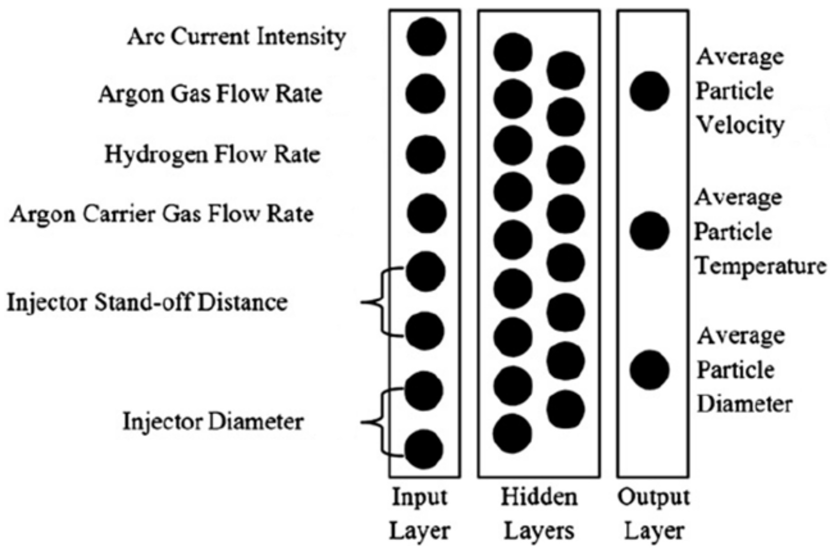

Figure 2. Supervised learning enables construction of nonlinear, multidimensional functional relationships between inputs and outputs of a complex system from experimental data, without prior assumptions about the nature of the relationships. Here, artificial neural networks were used to develop a data-driven model for predicting in-flight particle characteristics of an atmospheric plasma spray process for coating applications. The input–output model allowed for systematic analysis of the interdependencies and individual effects of the process parameters on the in-flight particle characteristics. Reprinted from [22], Copyright 2011, with permission from Elsevier.

of implicit information about the plasma characteristics [36, 37]. However, the information is often indirect, and generally requires computationally expensive analysis using physics-based models to extract physical quantities, e.g. gas temperature or concentration of reactive species [38].

Multivariate analysis techniques have been widely applied for process diagnostics in low-pressure plasma processing [24, 39, 40] and more recently in magnetically confined plasma fusion reactors [41, 42], but much remains to be done to more fully utilize ML for real-time and quantitative diagnosis of NEPs. A promising application of ML is inference of plasma characteristics from spectral information. Supervised learning methods as simple as linear regression can aid in inferring plasma properties such as neutral species rotational and vibrational temperature from raw optical emission spectroscopy data [6]. Such approaches can be viable alternatives to offline analysis of spectral data using more complex spectroscopic analysis models, and in turn enable rapid and real-time plasma diagnostics. Additionally, recording and analyzing the entire spectrum acquired from spectroscopy may be unnecessary and computationally expensive. Unsupervised learning methods for dimension reduction and multivariate analysis have proven useful for extracting latent information from spectral data, for example, using principle component analysis. Successful applications of unsupervised learning include identifying correlations between optical emission peaks and electrical properties or the estimated electron density of the plasma to investigate the discharge chemistry [10], and

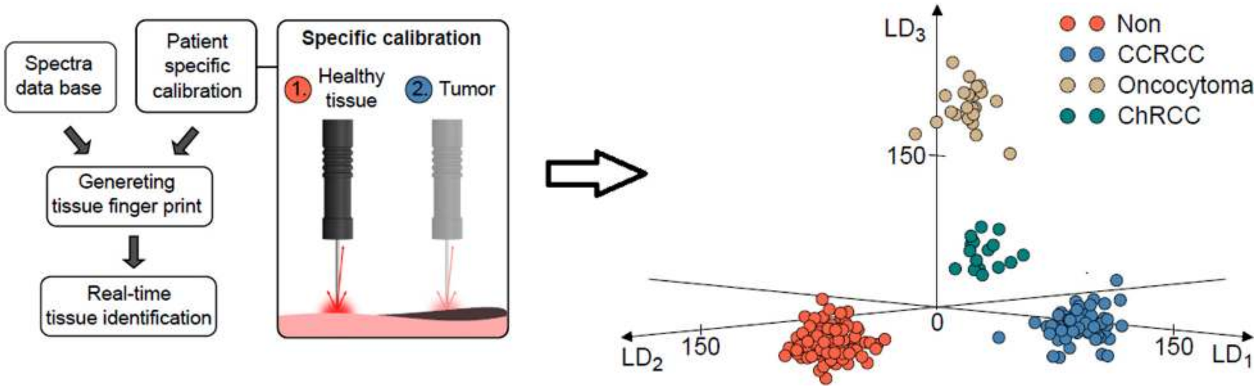

Figure 3. Supervised learning enables use of plasma diagnostics for inference of physical and chemical properties of complex surfaces interacting with the plasma in real-time. Here, a multi-class support vector machine was used to classify differences in the chemical composition of different tissue types based on high-resolution optical emission spectroscopy. Linear discriminant (LD) analysis was used to qualitatively visualize the classification results of tissue differentiation in low-dimension. Each point corresponds to a single optical emission spectroscopy measurement, where the color encodes the histological analysis of the measurement: healthy tissue (red points), clear cell renal cell carcinoma (CCRCC, blue points), oncocytomas (brown points), and chromophobe renal cell carcinoma (ChRCC, green points). The analysis indicated reliable differentiation between healthy and tumorous tissue in real-time. Reproduced from [32].

establishing the principal characteristic peaks of secondary ion mass spectroscopy to characterize the plasma-induced surface effects [43].

Machine learning also holds promise for inference of physical and chemical properties of complex surfaces interacting with NEPs that are often impractical to measure in real-time. There is generally an intricate interplay between the plasma characteristics and surface properties. Supervised learning would allow for deciphering the latent information of NEP diagnostics to detect and monitor variations in the chemical, electrical, or mechanical state of a surface. Time-evolution of the optical emission of NEP has been shown to provide useful information about surface properties [6, 44]. In [32], a multi-class support vector machine is trained for classification of differences in the chemical composition of different tissue types based on high-resolution optical emission of the plasma; see figure 3. Leveraging the fact that the emission of trace elements affects the tissue spectra, it is shown that the classification algorithm enables *in situ* differentiation of tumor from healthy tissue in real-time. Furthermore, unsupervised learning such as clustering of optical emission spectra may prove useful for detection of discrete surface changes, for example, in NEP processing of complex surfaces with highly nonuniform and heterogeneous electrical or thermal properties [6]; see figure 4.

Real-time process monitoring is another area where ML can play a pivotal role. For example, process monitoring can be important in detecting if the plasma has drifted from its proper operating regime. Reproducible operation of NEPs is generally susceptible to the intrinsic variability of plasma characteristics (e.g. due to long timescale drifts, or sharp spatial gradients in temperature and species concentrations) and high sensitivity to external disturbances (e.g. ambient humidity or temperature in atmospheric-pressure plasmas) [45]. Such variabilities in the NEP can be significantly aggravated when the plasma is brought in contact with a complex surface. Process monitoring

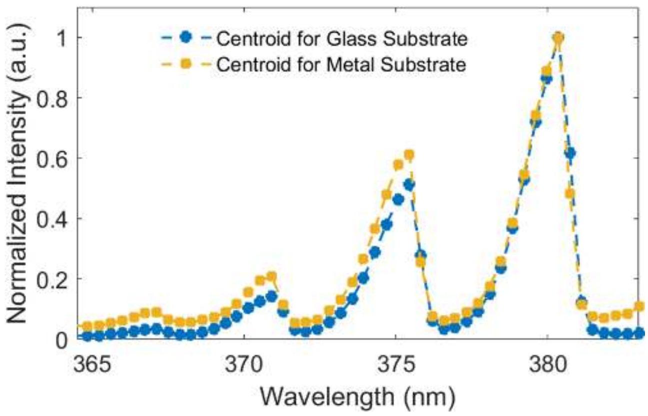

Figure 4. Unsupervised learning enables extracting the latent information in spectroscopy data for detection of discrete changes in properties of surfaces with heterogeneous characteristics. Here, *k*-means clustering was used to cluster the optical emission spectra of the second positive transition of N_2 obtained from a kHz-excited atmospheric pressure plasma jet in He into two classes corresponding to the glass and metal target substrates. The centroids—the average spectra—allowed for detection of the substrate type in real-time.

is crucial for timely detection of abnormal drifts and abrupt changes in the plasma characteristics such as a glow-arc transition. Successful monitoring relies on the ability to identify latent trends and correlations in information-rich data such as optical emission spectra, current–voltage signals, or electroacoustic emission measurements. ML has shown promise for developing data analytics capabilities that can decipher the latent information of on-line measurements to facilitate real-time diagnosis of plasma properties such as dissipated power, flow modes, and plasma mode transitions [6, 46–48]. Real-time process monitoring is indispensable for mitigating undesirable drifts or shifts in plasma properties and induced surface effects. Actively responding to these operational challenges requires real-time plasma process control [49].

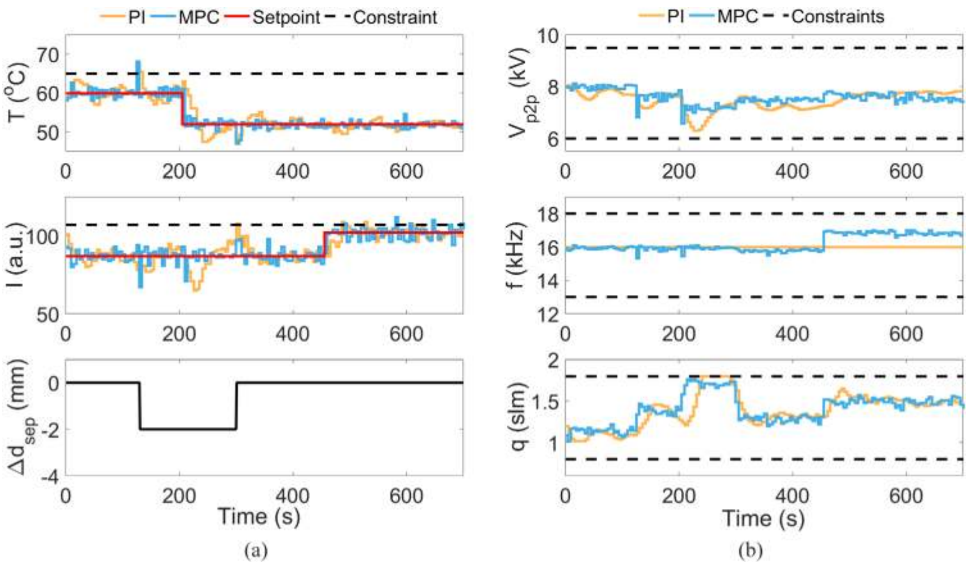

Figure 5. Unsupervised learning enables deriving low-dimensional, multivariable models of NEP dynamics for plasma process control over prespecified operating regimes. Here, the canonical variate analysis method was used to obtain a linear state-space model of the dynamics of a kHz-excited atmospheric pressure plasma jet in He targeted at a dielectric surface from input–output data. The process model was then applied to design proportional-integral (PI) control and model predictive control (MPC) strategies for the jet. The closed-loop control experiments showed the effectiveness of using model-based feedback control for setpoint tracking in the presence of a temporary step change of magnitude 2 mm in the device tip-to-surface separation distance Δd_{sep}. (a) Process outputs—maximum surface temperature T and total optical intensity of plasma I at the surface. (b) Manipulated process inputs—peak-to-peak voltage V_{p2p}, frequency of excitation f, and He mass flow rate q. © 2018 IEEE. Reprinted, with permission, from [45].

Machine learning for process control of NEP

Traditionally, control of NEPs has predominantly relied on statistical process control strategies, e.g. as widely adopted in semiconductor manufacturing processes [50]. Such control strategies are open-loop in nature, where the lack of on-line sensing and feedback corrective action can severely compromise the reliability and repeatability of NEPs due to the intrinsic plasma variabilities and external disturbances. It has been shown that model-based feedback control strategies are essential for repeatable and effective operation of NEPs, especially in safety-critical and high-performance applications [49, 51–55]. Some of the main challenges in feedback control of NEPs arise from (i) the complex, nonlinear interactions between multiple input and multiple output variables of a plasma discharge, (ii) the need to constrain the plasma properties such as voltage-current characteristics within admissible limits to circumvent undesirable phenomena such as mode transitions or adverse plasma-induced surface effects, and (iii) the need to maintain the proper synergy between the chemical, physical, and electrical effects of NEPs that interact with complex surfaces [54].

While it remains a significant challenge to derive physics-based models for NEPs that are adequately accurate and computationally efficient for process control applications, ML has shown promise for obtaining quantitative input–output models that are amenable to real-time computations. Unsupervised learning can be useful for obtaining low-dimensional, multivariable descriptions of NEP dynamics over prespecified operating windows of a process [45]; see figure 5. On the other hand, supervised learning, in particular neural networks, has emerged as a powerful means of modeling input–output

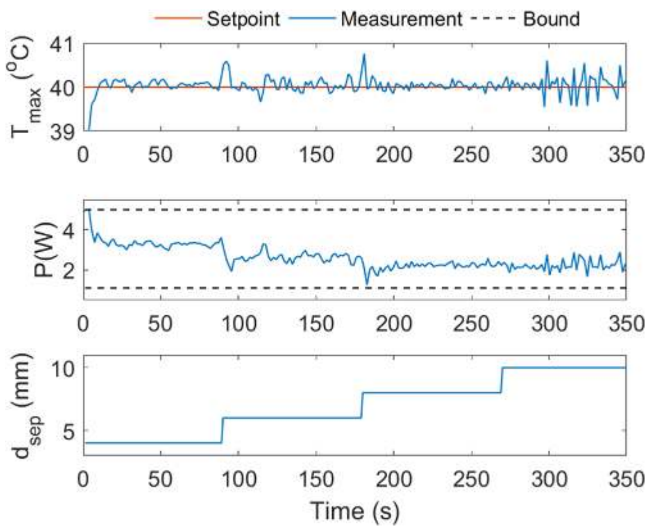

Figure 6. Reinforcement learning enables combining on-line learning and feedback control policy design for NEP applications subject to unknown variations in their behavior. Here, a reinforcement learning algorithm was trained using data from a kHz-excited atmospheric pressure plasma jet in He targeted at a dielectric surface. The goal was to maintain the maximum surface temperature (T_{max}) constant in the presence of step changes in the device tip-to-surface separation distance d_{sep} by manipulating the plasma power P. Real-time control experiments showed that the reinforcement learning algorithm was able to rapidly recover and maintain the maximum surface temperature at its desired setpoint after each step change in the device tip-to-surface separation distance. Adapted from [62].

mappings that have nonlinear character [56, 57]. The inherent ability of neural networks to learn complex mappings as well as the relative ease with which neural networks can be trained

Table 1. An overview of potential applications of ML for modeling, diagnostics, and control of NEPs.

	Supervised learning (e.g. regression, neural networks, kriging, support vector machines)	Unsupervised learning (e.g. clustering, dimension reduction)	Reinforcement learning
Predictive modeling	Learning nonlinear mappings for plasma-surface interactions [4, 22], learning inexpensive surrogate models from theoretical simulation data [7], plasma dose quantification	Selection of relevant input features for building simpler models from data [5]	
Diagnostics	Inference of plasma and surface properties from spectral data [6, 10, 32],	Extraction of latent information from measurements [46–48],	
	Detection of abnormal drifts and variabilities [6]		
Process control	Learning multivariable input–output mappings of process dynamics for model-based control [45, 56, 57]		Learning-based control

and adapted is likely to make them well-suited for nonlinear model-based control of NEPs. Model-based control strategies critically depend on accurate representations of the process dynamics. Neural networks can learn system responses from experimental data without prior knowledge of the system dynamics. This feature is especially useful when the fundamental understanding of the intricate interactions between the plasma and a complex surface is limited. Additionally, neural networks have the ability to deduce relationships from incomplete information, which can improve their tolerance to noisy or incomplete data. The availability of reliable models for describing NEP dynamics can pave the way for the widespread use of model-based control and optimization frameworks for controlling the synergistic effects of mass-momentum-energy exchange in various NEP applications [58]. Model-based feedback controllers can systematically accommodate the multivariable and nonlinear nature of plasma/plasma-surface dynamics, constraints on plasma variables that enforce various safety or performance requirements, and multiple, possibly conflicting, control objectives related to plasma-induced effects [49, 54].

Learning-based methods in control and artificial intelligence present another promising research area for NEP applications with complex dynamics and hard-to-model phenomena, where model-based control strategies with no on-line learning capability may have limited effectiveness [59]. In addition to alleviating the need for significant modeling and system identification effort, learning-based control can enable correction in anticipation of repeatable phenomena or external disturbances that cannot be modeled *a priori*; see figure 6. Reinforcement learning combines on-line learning and feedback policy design into a unified framework that provides a 'self-optimizing' feature via systematically balancing exploration (i.e. learning) and exploitation (i.e. feedback control) of an uncertain system [11, 60]. The advent of deep neural network architectures has transformed reinforcement learning applications by significantly increasing their real-time learning capabilities. Deep reinforcement learning has generated a considerable amount of excitement in the research community, especially in robotics applications with complex dynamics and uncertain environments [12, 61]. Such learning-based control approaches can potentially transform the way NEPs are operated today, especially when the plasma interacts with complex surfaces with time-varying and uncertain characteristics that in turn would lead to unpredictable plasma behavior and surface responses. Learning-based process control and artificial intelligence may become a critical component of future NEP applications, toward enhancing their reliability, flexibility, and effectiveness.

Concluding remarks

Table 1 summarizes our perspectives on some of the main areas where ML holds promise for transforming the current practice in modeling, diagnostics, and control of NEPs. Furthermore, ML and artificial intelligence may enable the development of modeling and simulation frameworks for NEPs that are self-aware and self-correcting; ideally, computer programs that are lifelong and never-ending learners [2, 63]. The availability of easy-to-use and open-source software such as TensorFlow, R, and scikit-learn is expected to accelerate widespread use of ML for NEP applications. Yet, developing reliable ML algorithms that generalize beyond their training data would depend on several critical issues, including: (i) systematic validation and cross-validation on independent datasets to avoid *overfitting* a model; (ii) use of some level of system knowledge or assumptions to improve the generalizability of a model beyond training data; (iii) selection of relevant input features to improve prediction accuracy and reduce computational cost of a model; and (iv) training and testing *model ensembles*, instead of a single model, to enhance reliability of predictions [64]. The field of ML is rapidly expanding, often via the invention of new ML problem formalizations that are driven by practical applications. The complex characteristics of NEPs, especially when interacting with complex surfaces in applications such as plasma catalysis or plasma medicine, may present unique challenges to the state-of-the-art ML methods and, thus, are expected to lead to development of specialized ML formalizations for NEPs. In our view, the paradigm of probabilistic or Bayesian ML, which enables quantifying and manipulating uncertainty about models and predictions [65], can play a central role in future developments of scientific data analysis and ML for NEPs. We envision that ML will become indispensable for addressing major science and technological challenges in NEPs in the years ahead.

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