Data Assimilation to Estimate the State of Partially Ionized Plasmas in Space Propulsion Systems

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KENTARO HARA and ANUBHAV DWIVEDI

ABSTRACT

Spacecraft electric propulsion plays a critical role in in-space missions. Understanding the state of the ionized gas, i.e., plasmas, is important for the characterization of thruster performance and the lifetime. In this talk, we present the recent development of data assimilation (DA) framework that estimates state variables and parameters obtained from a physics-based dynamical model with noisy experimental data. We have developed DA techniques based on variants of Kalman filters to estimate state and parameters in plasma systems governed by coupled nonlinear ordinary and partial differential equations.

INTRODUCTION

Spacecraft electric propulsion (SEP) typically use electrical energy obtained from solar panels and propellant stored in spacecraft to form energized gas that leads to thrust generation. The key metrics for SEP systems include thrust, specific impulse, thruster efficiency, and lifetime. There are three types of SEP systems, including electrothermal, electrostatic, and electromagnetic. In particular, the latter two types, i.e., electrostatic and electromagnetic thrusters, involved partially ionized gas, or also known as partially ionized plasmas. The gas flow is a mixture of positively charged ions, free electrons, and neutral gas. The positively charged ions are typically accelerated by electrostatic or electromagnetic forces, leading to a high exhaust velocity, i.e., high specific impulse. High specific impulse is beneficial for space missions as less propellant mass is required to achieve a given thrust, while the thrust of SEP systems is much lower than that of chemical propulsion systems.

The demand of SEP systems has significantly increased in the past decade. The main applications are orbit control and station keeping for geosynchronous satellite as well as low Earth orbit (LEO) satellite. For instance, Space-X's Starlink satellites carry a Hall effect thruster (HET), which is one of the most used SEP techniques in the market.

Kentaro Hara, Department of Aeronautics and Astronautics, Stanford University, 496 Lomita Mall, Room 252, Stanford, CA 94305, U.S.A.
Anubhav Dwivedi, Department of Aerospace and Mechanics, University of Minnesota Twin Cities, Minneapolis, MN 554544

In addition, SEPs have been used for deep-space missions, such as sample return by Hayabusa and Psyche. While such propulsion devices have been used for in-space missions, optimization of the thruster design and on-orbit control has significant room for improvement. It is critical to advance the understanding of the complex plasma phenomena to control and optimize the thruster operation.

While various physics-based models, such as fluid and kinetic models [1], have been developed to model complex physical and chemical processes of partially ionized plasmas, data-driven models have recently gained attention. The primary motivation for pursuing data-driven models stems from (a) desire to better utilize measurement data to infer the state and health of the SEP system, and (b) the inherent complexity of plasma physics, particularly due to significant uncertainties in collisional and transport processes. Various volumetric reactions occur simultaneously, including elastic and inelastic collisions between multiple species, which are characterized by the rate coefficients (rate constants). In addition, plasma-material interaction is complex since the ions, electrons, and radical species interact with various types of materials, including conductors and insulators, resulting in phenomena such as electron emission, erosion, and thermal accommodation. Hence, even if we have the perfect physics-based model with the sufficient fidelity, there are uncertain parameters that may affect the multiscale dynamics (e.g., due to plasma oscillations from GHz to kHz).

The alternative approach is to develop a data-driven modeling framework. Instead of conventional machine learning tools that investigate the correlation between data streams, data assimilation (DA) is a unique framework that combines both the physics-based model and the experimental data, i.e., measurement data. The states and parameters can be estimated through a sequential or variational DA framework. The goal of such DA methods depends on the application. For instance, for weather forecasting, the primary goal is to predict the weather. In other instances, the DA framework might be used to control the dynamics of a system (e.g., robots). Here, we apply the DA framework to infer the unknown parameters that are difficult to be measured in the plasma system.

DATA ASSIMILATION FOR PARTIALLY IONIZED PLASMAS

Figure 1 shows the basic idea of the Kalman filters. The estimated state variables and parameters in the system will be evolved according to the physics-based dynamical model (Forecast phase). When measurement data are available, the probability density function (PDF) of the estimated state variables and parameters can be updated (Analysis phase) [2]. The main reason why we are interested in sequential DA using Kalman filters is because of the spatio-temporal estimation of the state variables and parameters as spatially and temporally varying measurement data become available. The forecast phase can be generally described as

$$d\boldsymbol{u}/dt = f(\boldsymbol{u}) + Gw, \tag{1}$$

where $\boldsymbol{u}$ is the state variables, which can include parameters, f is the dynamical function, G is the process noise gain, and w is the process noise. The measurement data can be written as

$$\boldsymbol{y}_k = h(\boldsymbol{u}_k) + \boldsymbol{v}_k, \tag{2}$$

where $\boldsymbol{y}$ is the measurement data set, h is the observation function, and $\boldsymbol{v}$ is the measurement noise. The subscript k indicates the discrete time that the measurement data are available.

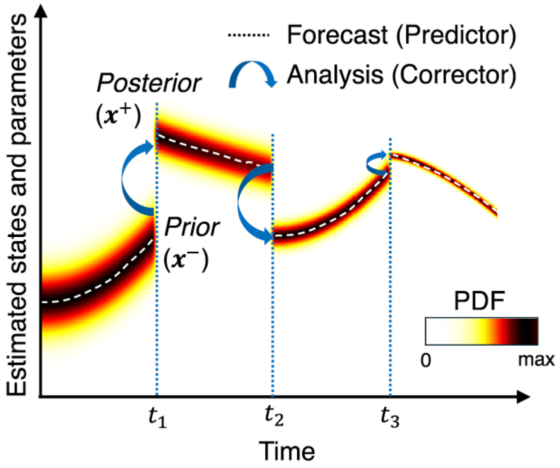

Figure 1. Illustration of Kalman filters updating the probability density function (PDF) of the state and parameter estimation [Reproduced from Ref. 3]

There are several variations of the Kalman filter family, including extended Kalman filter (EKF), ensemble Kalman filter (EnKF), unscented Kalman filter (UKF), and particle filter (PF). The main difference between such methods is how to capture the propagation of the PDF in the forecast phase. For instance, EKF solves for the transport equations of the mean estimation as well as the covariance of the associated uncertainty of this estimate. Linearization about the mean state is used for propagating the covariance which can be computationally demanding. Instead, EnKF considers the propagation of various instances of the nonlinear dynamics which are gathered to construct the PDF. The initial PDF is represented by M ensembles, which are propagated by the physics-based model. When the measurement data are available, the M ensembles are used to calculate the mean estimation and covariance to update the individual instances.

EXAMPLES

In this paper, we present our two recent examples: (1) EnKF of a 0D collisional radiative model where optical emission spectroscopy (OES) data are used [3]; (2) EKF of a 1D plasma PDE model where laser induced fluorescence and time-varying discharge current are used as measurement data [5].

Figure 2 shows a schematic of the physical and chemical processes that occur in low-temperature plasmas (LTPs), where electrons, ground state neutrals, radicals, and ions can interact with each other. Some radical states also emit radiation when deexcitation occurs. Hence, the model that captures the collisional and radiative processes is called the collisional-radiative model (CRM). The state variables evolve in time. Using various measurement techniques, one can infer the state variables of the partially ionized plasmas. In Ref. 3, we have demonstrated using the EnKF that combines a 0D CRM with OES data, which measure the radiative quenching of radical species emitting photons with discrete frequencies associated with the energy levels. Typically, a forward simulation requires running the physics-based CRM for a long time resolving the necessary time scales (e.g., the fastest reactions may be on the order of GHz, while the slowest ones may be on the order of kHz or Hz). Once steady state is achieved in the physical model, the simulation data are collected and compared with experimental data for validation. On the other hand, an inverse calculation using EnKF utilizes the measurement data directly while advancing the 0D CRM, allowing for fast estimation of the hidden parameters, here the electron energy distribution function (EEDF).

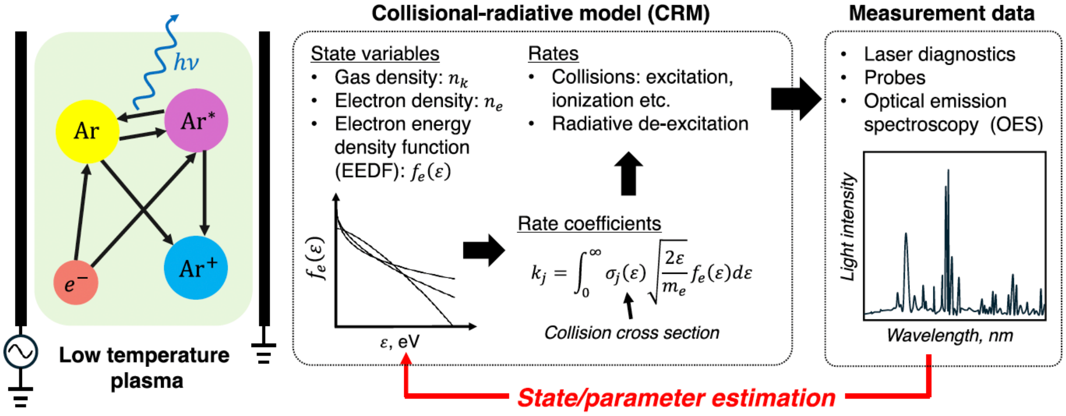

Figure 2. Using EnKF to estimate the electron energy distribution function (EEDF) [Reproduced from Ref. 3].

Another example of the DA framework is the 1D predator-prey dynamics of partially ionized plasmas in a HET. The governing equations of this test case are the ion and neutral atom continuity equations, which are both PDEs.

$$N_t = -(NU)_x + N\,n\,k_i(T_e) \tag{3}$$

$$n_t = -(nu)_x - N\,n\,k_i(T_e) \tag{4}$$

where N and n are the number densities of the ions and neutral atoms, U and u are the bulk velocities of the ions and neutral atoms, respectively, k_i is the ionization rate coefficient as a function of the electron temperature, T_e, and subscripts t and x denote the temporal and spatial derivatives, respectively. The ionization rate coefficient that we use follows Ref. 4. We consider a measurement dataset obtained for a SPT-100 HET in Ref. 5. Laser induced fluorescence (LIF) is used to measure the spatio-temporal profile of the ion velocity distribution function during a 20 kHz breathing mode oscillation. In addition, the discharge current is a function of time.

We developed an EKF that use the 1D predator-prey model in Eqs. (3) and (4) and the measurement data to infer the electron temperature as a function in space and time. In the EKF, we have used two numerical treatments. One is the spatially correlated noise, which was found to be important to handle the numerical errors due to both the physics-based model (e.g., truncation error) and the measurement error. The other is a parameter covariance regularization. Because in the EKF, there is no transport equation associated with the parameters, the covariance of the parameters is dictated by the

Kalman gain process. We observed that without the regularization, the parameter estimation does not reach steady state. Figure 3 shows an example of the PDE state and parameter estimation. Using spatio-temporal profile of the LIF data and time-varying discharge current, we successfully obtained the estimation of the ion density, neutral density, and electron temperature. [6]

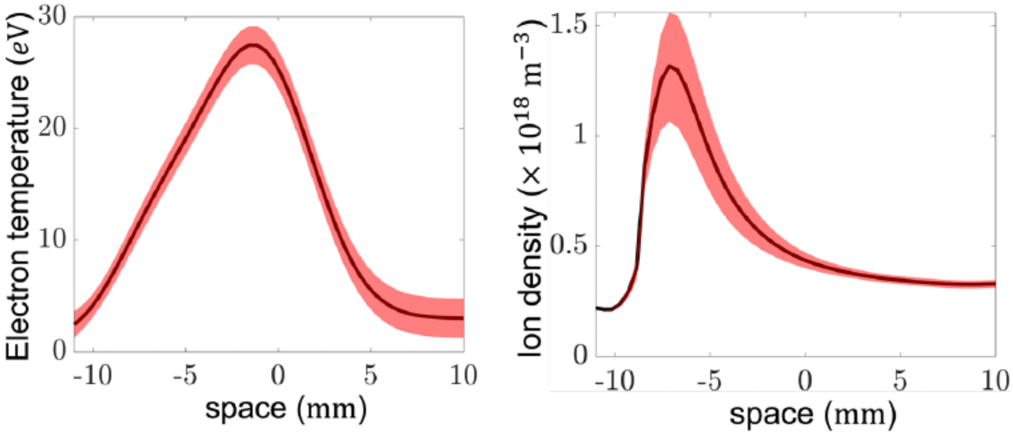

Figure 3. EKF of 1D PDE describing the predator-prey dynamics [6].

SUMMARY

We have developed various DA framework for understanding the state variables and parameters of partially ionized plasmas that are used in spacecraft electric propulsion. The EKF and EnKF models are applicable to a wide range of dynamical systems.

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