Physics assisted Latent Space Dynamics Learning for Stiff Collisional-radiative Models

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Collisional-radiative (CR) models describe the atomic processes in a plasma by tracking the population density in the ground and excited states for each charge state of the atom/ion. These models predict important plasma properties such as charge state distributions and radiative emissivity and opacity. Accurate descriptions of the CR balance of the plasma are essential in fusion whole device modeling, especially when significant impurities are introduced into the plasmas. In an integrated fusion plasma and CR simulation, a CR model is mathematically represented as a high-dimensional parameterized stiff ODE:

$$\frac{d\mathbf{N}}{dt} = R(\mathbf{N}; n_A, T_e)\,\mathbf{N}, \tag{1}$$

with $\mathbf{N}$ the population density of ions in various charge states, R is the rate matrix, T_e is the temperature, n_A is the total density for species. The state-of-the-art CR models contain orders of millions degrees of freedom and can take hours to obtain a solution. It is simply impossible to directly couple the CR physics module in its original form to 3D plasma simulations, since for each spatial grid point in the plasma simulation, one would need to evolve a coupled ODE with 10^{3-6} degrees of freedom, which would overwhelm the plasma simulation cost by many orders of magnitude. The goal of this work is to introduce a reduced-order model that can efficiently and accurately predict the fast scale dynamics transition of the charge state, $n_{\alpha,Z}$, and the radiative cooling rate, $\mathscr{R}_L$.

The main challenge in finding the reduced CR model lies in two parts. The first is to efficiently identify the low-dimensional representation from the data that can recover the small fast scale in the full system. The second is to learn latent dynamics that can accurately predict the trajectories of the reduced system using only the initial conditions. This allows for an approximation of the full-order dynamics and radiative cooling rate with high accuracy. Fig. 1 plots the trajectories of different charge states from the high-fidelity numerical simulation. It is evident that the sharp transitions over very short time scales present a significant challenge in accurately modeling the reduced CR dynamics. In this work, we introduce a novel physics-assisted latent space dynamics

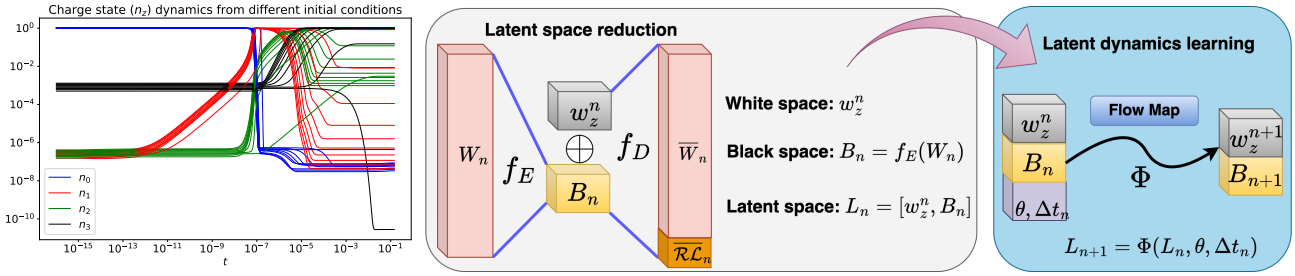

Figure 1: Left figure: Trajectory of the charge state from the high-fidelity numerical simulation of the CR model for different initial conditions. Four colored lines represent four charge states (they are partial sums of the solution state vector; details will be defined later), n_0, n_1, n_2, n_3. A fast transition of the dynamics at a tiny time scale (10^{-7}) can be observed. Right figure: Model architecture for physics-integrated latent space identification. Flow map network for latent dynamics learning. θ denotes the parameter space in our CR system which are total density, n_A, and temperature, T_e.

learning approach based on deep neural networks. First, we use an autoencoder neural network to identify the low-dimensional representation of the original high-dimensional CR system. This representation is denoted as the black space. We then incorporate the known physical information, specifically the charge states, denoted as the white space, into the entire latent space. *This gray-box approach ensures that both data-driven and physics-based aspects are integrated into the model.* Then, we use a flow map neural network to learn the dynamics within the latent space. To the best of our knowledge, this is the first effort to apply the integrated data-driven and physics-based latent dynamics learning for constructing a reduced-order model of a parameterized CR system. For the purpose of demonstration, our approach is tested by the CR data from a single species, lithium, under different parameters and initial conditions. Numerical experiments reveal that our model can efficiently and accurately predict the true dynamics of the CR system.