Abstract

An integrated-modeling workflow has been developed to predict equilibria and response to 3D magnetic perturbations in tokamak experiments. Starting from an equilibrium reconstruction from a past experiment, the workflow couples together the EFIT Grad-Shafranov solver, EPED model for pedestal structure, and NEO drift-kinetic-equation solver (for bootstrap current calculations) in order to generate equilibria with self-consistent pedestal structures as the plasma shape and various scalar parameters (e.g., normalized $\beta$, pedestal density, $q_{95}$) are changed. These equilibria are then analyzed using automated M3D-C1 to compute the MHD plasma response to 3D magnetic perturbations. The workflow was created in conjunction with a DIII-D experiment studying the effect of triangularity on plasma response, showing excellent agreement between the analysis of the workflow’s equilibria and equilibria reconstructed from the experiment. A predict-first study was then carried out for a DIII-D experiment examining how plasma response varies between single- and double-null shapes. The predicted equilibria were used to guide experimental planning and the predicted response was found to agree well with the perturbed magnetic field measured on the high-field-side midplane, including some unexpected trends. Another predict-first study of high-$\beta_p$ discharges in DIII-D found that the plasma response was very small unless $q_{95}$ was lowered to values significantly below those typically run in such plasmas. This result potentially explains the difficulty of achieving ELM suppression in high-$\beta_p$ discharges. Finally, a new workflow based upon individual steps for different codes/models that all read from and write to a centralized data structure is discussed. The increased flexibility of this new workflow makes it an ideal candidate for performing predictive scenario development across current and future devices (e.g., ITER).
1. INTRODUCTION

Predictive modeling is frequently used to inform present-day tokamak research, optimizing experiments by identifying useful actuators and diagnostics. Furthermore, such modeling has been used to identify new physics to explore experimentally (e.g., the prediction and subsequent observation of Super H-mode [1, 2]). The role of predictive modeling will increase dramatically in the coming years to ensure the successful design and operation of future tokamaks, such as ITER. The immense thermal and magnetic energies stored in larger tokamaks greatly increase the risk of machine damage during off-normal events. These tokamaks will be unable to explore all the physics of disruptions, edge-localized mode (ELMs), and divertor heat fluxes experimentally. Thus, high-fidelity predictions based on sophisticated theory and integrated models are required and must be validated against present-day experiments.

Many theoretical and numerical models that are capable of predicting results from experiments require inputs determined post-experiment to achieve agreement. For example, linear MHD codes have predicted experimental stability limits accurately, but use experimental equilibrium reconstructions as input [3, 4]. A “predict-first” paradigm, while more challenging, has several advantages. First, predictions made in-advance of a specific experiment can be used to guide experimental planning and execution. Second, predict-first studies require an accurate accounting of uncertainties in both the upcoming experiment and in the models used, preventing the possibility of fine-tuning simulations to achieve agreement. Third, predict-first is more applicable to the study of future devices, for which no experimental results yet exist.

Here, progress is presented on integrated-modeling workflows meant to allow predict-first simulations of present-day and future tokamaks. Section 2 provides a review SEGWAY, a recently published [5], predict-first, integrated-modeling workflow. Starting with an equilibrium reconstruction from a past experiment, SEGWAY couples together the several codes in order to generate equilibria with self-consistent pedestal structures as the plasma shape and scalar parameters (e.g., normalized $\beta$, pedestal density, edge safety factor $\langle q_{95} \rangle$) are changed. These equilibria can then be analyzed just like experimental equilibrium reconstructions. In Section 3, two new predict-first studies are presented and compared to experimental results where available. Finally, in Section 4, a new, more-powerful, more-flexible predict-first workflow that is under active development is presented and the future of predict-first, whole-device modeling is discussed.

2. BACKGROUND

The Self-consistent Equilibrium Generation Workflow for AnaYsis (SEGWAY) [6] was developed using the OM-FIT integrated-modeling framework [7, 8] in order to predict equilibria in upcoming tokamak experiments. SEGWAY uses a similar paradigm to that used in experimental tokamak research, namely, begin with an existing target plasma, prescribe a change to the plasma (e.g., shape) while fixing other constraints (e.g., $N$), and analyze the resulting effects of that actuator on the plasma. To do this numerically, SEGWAY iterates through several codes and modules until a self-consistent equilibrium is obtained that satisfies all required constraints. In Section 2.1, the workflow implemented in SEGWAY is briefly described. In Section 2.2, results from applying SEGWAY to a DIII-D triangularity-scan experiment are shown. Note that both the workflow and comparison to this particular experiment were previously published in Ref. [6], which will not be further extensively cited.

2.1. Description of SEGWAY

SEGWAY begins with a high-fidelity equilibrium from an existing tokamak experiment that has been reconstructed using magnetics data, safety-factor profiles from motional-Stark-effect (MSE) diagnostics, and measurements of the density, temperature, and rotation profiles. The SEGWAY workflow published in Ref. [6] then takes in target values for the plasma shape (e.g., elongation $\kappa$, triangularity $\delta$) along with $\beta_N$, the edge safety factor $\langle q_{95} \rangle$, and the electron pedestal density $n_{e,ped}$. An updated version of SEGWAY which will be used in Section 3.1 also allows the user to specify a desired plasma boundary shape as an $(R, Z)$ array of points. SEGWAY then uses the EFIT Grad-Shafranov solver [9, 10, 11] to recompute the equilibrium with the desired shape. EFIT itself is iterated upon, changing $p'$ and $f f'$ in order to achieve a desired pressure and current profile. Given the new
equilibrium, the pressure profiles is modified in two ways. First, the height and width of the pedestal pressure are scaled according to EPED1-NN [12], neural nets trained to the EPED1 model [13, 14]. EPED1 uses a simple set of scalar inputs in order to predict the height and width of the pressure pedestal based on the criticality to peeling-ballooning and kinetic-ballooning modes. EPED1-NN reproduces the EPED1 results to within roughly 10% with a billion times speedup. Second, the core pressure profile is scaled using a simple analytic formula in order to target the desired $\beta_N$. After the new pressure profile is computed, the underlying density profiles are uniformly scaled such that the desired $n_{e,\text{ped}}$ is achieved and the temperature profiles are scaled to be consistent the densities and pressure. Then, the NEO drift-kinetic equation solver [15, 16] is used to calculate a new bootstrap current profile. An “ohmic” current profile is computed by subtracting away the old bootstrap current. This ohmic current is then scaled with a simple analytic formula and the new bootstrap current added to it, with the ohmic scaling determined by the desired $q_{95}$. After this single SEGWAY cycle, there is a new equilibrium, pressure profile, and current profile, but there’s no guarantee that they are consistent with each other. Thus, SEGWAY is iterated until self-consistency and all the desired target parameters are achieved. This is shown schematically in Figure 1.

The resulting SEGWAY equilibria have all the information necessary to perform the same analysis that would typically be performed after an experiment using reconstructed equilibria. In particular, the M3D-C1 extended-MHD solver [17] is used to compute linear stability and/or linear plasma response to 3D magnetic perturbations. Such analysis is appropriate to experiments on the avoidance and control of transient MHD events, such as disruptions and ELMs.

2.2. Validation with DIII-D Triangularity-Scan Experiment

SEGWAY was originally developed in conjunction with a DIII-D experiment studying the effect of triangularity on the plasma response to $n = 3$ magnetic perturbations, along with the resulting effects on ELM suppression. A predict-first study was initially carried out using a reduced version of SEGWAY, which lacked the coupling to NEO and constraints on $\beta_N$. Despite these missing physics, these predicted equilibria helped to guide the experiment by identifying the plasma current required to hold $q_{95}$ fixed as the triangularity was varied. The full SEGWAY model was then developed as experimental analysis progressed. With the inclusion of the bootstrap current and $\beta_N$ constraints, it was found that M3D-C1 plasma-response analysis of the SEGWAY equilibria was in excellent agreement with the same analysis performed on high-fidelity equilibrium reconstructions from the experiments. Figure 2 shows the magnitude of the magnetic perturbations induced by the plasma response on the low-field-side (LFS) and high-field-side (HFS) midplane of DIII-D. The responses computed by M3D-C1 for the SEGWAY and reconstructed equilibria are in quantitative agreement across all triangularities considered. Thus, SEGWAY was shown to generate equilibria that accurately represent reconstructed equilibria, for the purpose of this analysis, giving us confidence in applying SEGWAY forward for true, predict-first studies, as described in Section 3. Note that extensive details on the various workflows used as SEGWAY was developed, along with a comparison to the experimentally measured plasma response can be found in Ref. [6].
3. PREDICT-FIRST ANALYSIS WITH SEGWAY

3.1. Plasma response in single- and double-null plasmas

SEGWAY was used to perform a predict-first study for a DIII-D experiment exploring the plasma response to 3D magnetic fields in single- and double-null plasmas. Previous limited experiments had shown that double-null plasmas tended to have decreased plasma response, particularly on the high-field side of the tokamak, which correlated with a loss of ELM suppression [18]. This updated experiment sought to do detailed scans between matching single- and double-null plasmas by varying $dR_{sep}$, the radial distance at the outboard midplane between the magnetic surfaces connected to the lower and upper X-points. Note that $dR_{sep}<0$ is lower single null (LSN), > 0 is upper single null (USN), and = 0 is double-null (DND).

A set of nine plasma boundaries were constructed in the range $dR_{sep} = [-4 \text{ cm}, 4 \text{ cm}]$ by the linearly superposition of boundaries from existing equilibrium reconstructions of one LSN plasma (DIII-D shot 146065) and one DND plasma (DIII-D shot 146058). Then, beginning with the reconstruction of shot 146065, SEGWAY was run for each boundary (using EFIT as a fixed-boundary solver) and maintaining constant $q_{95}$ = 4.1, as was going to be targeted in the experiment. As in the triangularity-scan experiment of Section 2.2, the predicted equilibria were used to help guide experimental planning, particularly providing the plasma current required to maintain constant $q_{95}$ as $dR_{sep}$ was varied. Due to expected uncertainty in some other experimental parameters, SEGWAY was run four times for each boundary, for each combination of $\beta_N = 1.8$ & $2.0$ and $n_{e,ped} = 2 \times 10^{19}$ & $3 \times 10^{19}$ (a total of 36 different equilibria).

Each SEGWAY equilibrium was analyzed before the experiment using automated M3D-C1 in order to predict the linear plasma response to both $n = 2$ and $n = 3$ even-parity magnetic perturbations. Figure 3 shows the M3D-C1 predicted plasma response at the DIII-D low-field-side midplane (LFS) and two high-field-side midplane locations (HFS-A, just above midplane, and HFS-B, just below). Since neither $\beta_N$ nor $n_{e,ped}$ were well-constrained in the experiment, the predicted response over the equilibria with each combination of $\beta_N$ and $n_{e,ped}$ were averaged (with appropriate error bars) at fixed $dR_{sep}$. It was predicted that, while the LFS response would show little variation with $dR_{sep}$, there would be definite variation on the HFS. Of particular interest was an unexpected asymmetry, with the USN HFS prediction’s generally being significantly higher than the LSN HFS prediction. It was also predicted that, with the exception of $n = 2$ HFS-B, the HFS response would not necessarily be minimized in the DND configuration.

The measured plasma response from the subsequent experiment is also plotted in Figure 3, with the $n = 2$ data taken from shot 173806 and $n = 3$ from 173817. While the LFS predictions showed poor quantitative agreement with the measurements, the predicted lack of strong variation with $dR_{sep}$ was observed. The predicted HFS responses, on the other hand, showed general quantitative agreement with the measurements. In addition, qualitatively, the asymmetry of the HFS response between LSN and USN (particularly for HFS-A) and the lack of a HFS...
null-response in the DND configuration were seen in both the predictions and the experiment. While the fine-scale structure of the response was not consistently seen in the predictions, this is likely due to the sparsity of the \( dR_{sep} \) values simulated by SEGWAY.

### 3.2. Impact of \( q_{95} \) on plasma response in joint EAST/DIII-D High-\( \beta_p \) experiments

A joint task force between EAST and DIII-D has extensively studied the physics of high-poloidal-\( \beta \) (\( \beta_p \)) plasmas [19]. A recent experiment on DIII-D sought unsuccessfully to establish ELM suppression in such plasmas, which featured a double-null configuration, high \( q_{95} \), and internal transport barriers (ITBs) leading to relatively high core pressures. SEGWAY was used to vary parameters in high-\( \beta_p \) plasmas, seeking to use M3D-C1 analysis to understand why ELM suppression was not achieved.

Beginning with an equilibrium reconstruction of \( 170361 \) (\( q_{95} = 6.34, \beta_N = 2.99, \) and \( \beta_p = 1.84 \)), SEGWAY was run targeting 14 different \( q_{95} \) values ranging from 3.4 to 10.4, while holding \( \beta_N \) and the plasma shape fixed. Each predicted equilibrium was then analyzed using M3D-C1 to calculate linear \( n = 3 \) plasma response. It was found that the plasma response was only significant for \( q_{95} \lesssim 5.4 \), well-below the experimental value. Figure 4 shows the single-fluid, even-parity, resonant magnetic perturbation (vacuum and vacuum-plasma response) at the magnetic surface in each equilibrium that had the greatest resonant penetration. This decreasing response with \( q_{95} \), however, is true for both single- or two-fluid modeling, even- or odd-parity vacuum fields, and resonant or non-resonant response. Further investigation of these simulations revealed that the decrease is correlated with neither the magnitude of rotation at the rational surface nor the magnetic shear. The physics cause for the decreased response at high-\( q_{95} \), therefore, remains an area of ongoing study.

The investigation of both past and future experiments on both DIII-D and EAST that could be used to validate this prediction is an area of ongoing research. ITBs, a hallmark of high-\( \beta_p \) discharges, are difficult to maintain at lower-\( q_{95} \) due to there being a minimum required \( \beta_p \approx 1.9 \approx \beta_N q_{95} \) for sustaining ITBs in the scenario [20]. Thus, this prediction suggests that it may be challenging to achieve ELM suppression in high-\( \beta_p \) plasmas with ITBs.
Figure 4: The maximum resonant field in the edge as a function $q_{95}$ at constant $\beta_p \approx 2.99$, as computed by M3D-C1 for SEGWAY-generated equilibria based on high-$\beta_p$ plasmas. Significant resonant amplification only occurs for $q_{95}$ well-below the experimental value.

Nevertheless, SEGWAY provides a valuable tool for studying other parameters that could be tuned to increase the plasma response in high-$\beta_p$ discharges, thus increasing the likelihood of achieving ELM suppression.

4. CONCLUSIONS AND THE FUTURE OF PREDICT-FIRST, WHOLE-DEVICE MODELING

SEGWAY has proven to be a useful tool for predict-first modeling of present-day experiments. Developed alongside a DIII-D experiment studying the effect of triangularity on plasma response to 3D magnetic perturbations, the M3D-C1 analysis of SEGWAY-generated equilibria and experimental reconstructions showed remarkable agreement. SEGWAY was then used to predict the plasma response in DIII-D single- and double-null plasmas, showing fair quantitative agreement with measured magnetic signals on the tokamak HFS. Several unexpected, qualitative features seen in the predictions were also found in the experiment (Figure 3). As part of the a joint EAST/DIII-D task force, SEGWAY was also used to predict that the plasma response should almost disappear at the high-$q_{95}$ values typically operated at in high-$\beta_p$ plasmas. Further study with SEGWAY is necessary to inform experiments about the most promising directions to investigate for increasing the plasma response and achieving ELM-suppression in high-$\beta_p$ discharges.

SEGWAY’s reliance on existing equilibrium reconstructions and simple scalings therefrom restricts the workflow to generating equilibria that are somewhat similar to plasmas that have already been produced from experiments. In addition, SEGWAY was created to capture phenomena most relevant to pedestal evolution. Extending it to improve the fidelity of predicted core and edge phenomena, while planned, may prove cumbersome due to the rigid structure of the workflow. For predict-first, whole-device modeling in future tokamaks, a more powerful and more flexible tool is necessary.

To this end, the development of a new OMFIT workflow called STEP (Stability, Transport, Equilibrium, and Pedestal) has been undertaken, a schematic for which is shown in Figure 5. Unlike SEGWAY which transfers data directly from code to code, STEP uses ITER Integrated Modeling & Analysis Suite (IMAS) [21] Interface Data Structures (IDSs) as universal repositories for all simulated data in the workflow. For each code, a “step” is created that reads all necessary input information from the IDSs, runs the code, and then writes the output back to the IDSs. To assist with the interfacing to the IDSs, STEP makes extensive use of the new Ordered Multidimensional Array Struture (OMAS) python library [22]. Table 1 provides a list of existing and planned steps for various codes.

This system of steps and a centralized repository offers several advantages over circular, code-to-code workflows. First, desired steps can be run in arbitrary order, allowing for the flexible design of workflows to suit individual needs. Second, it allows for the simple addition of new steps, as each code only needs to interface with OMAS, not every other code individually. Third, STEP can start from any number of initial conditions, including experimental data or a simple, predicted configurations for future tokamaks (e.g., ITER). So long as sufficient information to
Figure 5: Schematic representation of the STEP workflow. Each step exchanges inputs and outputs with a central repository using OMAS.

Table 1: Available steps and their inputs and outputs. The SEGWAY step implements the scalings of experimental profiles from the SEGWAY workflow. †Magnetic topology (MT). *Planned.

run a given code is already stored in the IDSs, a step can be taken.

Currently, several standard workflows are being developed and tested. One example would be to use the ONETWO transport solver [23, 24], EFIT, and the TGYRO (TGLF quasilinear turbulence [25] and NEO neoclassical) transport solver [26] to evolve the plasma sources, current, equilibrium, and kinetic profiles self-consistently. These steps can be iterated upon in an open loop (e.g., given fixed injected power, predict an equilibrium and associated profiles) or, using an optimization wrapper that has been implemented, a closed-loop (e.g., given a desired $N$, predict the injected power needed). By including MHD stability steps (e.g., the ideal MHD code GATO [27]), a plasma-stability manager can be created, feeding back on various actuators to ensure plasma stability. Such workflows will be invaluable for planning experiments on current devices and predicting performance and appropriate scenarios in future tokamaks like ITER.

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