ADAPTIVE MODEL REFINEMENT FOR THE IONOSPHERE AND THERMOSPHERE

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ABSTRACT. Mathematical models of physical phenomena are of critical importance in virtually all applications of science and technology. This paper addresses the problem of how to use data to improve the fidelity of a given model. We approach this problem using retrospective cost optimization, a novel technique that uses data to recursively update an unknown subsystem interconnected to a known system. Applications of this research are relevant to a wide range of applications that depend on large-scale models based on first-principles physics, such as the Global Ionosphere-Thermosphere Model (GITM). Using GITM as the truth model, we demonstrate that measurements can be used to identify unknown physics. Specifically, we estimate static thermal conductivity parameters, and we identify a dynamic cooling process.

1. INTRODUCTION

The goal of this work is to use data to build better models. Figure 1 illustrates this objective. Models serve a variety of purposes by capturing different phenomena at varying levels of resolution. High-resolution models are desirable when the goal is to understand scientific phenomena or assimilate data, whereas a coarser model may be preferable when the goal is to capture critical details in an efficient manner, for example, for fast prediction or control. Consequently, the fidelity of a model must be gauged against its intended usage.

![Figure 1](image)

Figure 1. This diagram illustrates the goal of this work, namely, initial model + data = improved model.

Most models are constructed from collections of interconnected subsystem models, which in turn are based on a combination of physical laws and empirical observations. For example, the core of a model might be the Navier-Stokes or MHD equations, while various source terms (such as chemistry, heating, and friction) may be modeled using either first principles

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submodels or empirical relations that have different levels of self-consistency and complexity. Physical laws embody first-principles knowledge, whereas empirical observations may include relations that are based on the statistical analysis of data, for example, regression. Physics can provide the backbone of a model, while empirical relations can flesh out details that are beyond the ability of analytical modeling (e.g., sub-grid-scale phenomena).

When data are available, an empirical model can be constructed by means of system identification methods. The construction of a linear dynamic model that relates measured inputs to measured outputs is well developed [14, 15, 16]. A more challenging problem is to develop methods for nonlinear system identification. Since nonlinear models can have a vast range of structures, the problem of nonlinear system identification requires the choice of a suitable model structure as well as an algorithm that uses data to tune the parameters of the model. Model structures range from black-box (unstructured) models, such as neural networks, to grey-box and white-box models, where some or all of the structure of the model is specified [17, 18, 19, 20].

Accessibility impacts the ability to perform nonlinear model identification. For example, the Hammerstein and Wiener grey-box model structures, in which a static nonlinear mapping is cascaded with a dynamic linear subsystem, are reasonably tractable for model identification [21]. However, when the static nonlinear mapping of a dynamic linear system is not directly accessible, in the sense that neither its input nor its output is directly measured, then the identification problem becomes significantly more difficult. The highest degree of accessibility arises when two variables are measured and the unknown subsystem is a static mapping between the variables.

System identification is typically concerned with the construction of a model of the entire system. In contrast, our goal is to identify a specific subsystem of the model, where the remainder of the model is assumed to be accurate and the goal is to improve understanding of the physics of the poorly modeled subsystem despite its low accessibility. With this concept of accessibility in mind, we introduce the problem of data-based model refinement, where we assume the availability of an initial model, which may incorporate both physical laws and empirical observations. The components of the initial model may have varying degrees of fidelity, reflecting knowledge or ignorance of the relevant physics as well as the availability of data. With this initial model as a starting point, our goal is to use additional measurements to refine the model. Components of the model that are poorly modeled can be updated, thereby resulting in a higher fidelity model, as shown in Figure 1. This problem is variously known as model correction, empirical correction, model refinement, model calibration, or model updating, and relevant literature includes [1, 2, 3, 4] on finite-element modeling, [5, 6, 7] on meteorology, [8] on feedback control, as well as our algorithmic research [9, 10, 11] with applications to health monitoring [12, 37].

The uncertain physics of a subsystem may range from the simplest case of an unknown parameter (such as a diffusion constant), to a multivariable spatially dependent static mapping (such as a conductivity tensor or boundary conditions), to a fully dynamic relationship among multiple variables (such as reaction kinetics). The difficulty of identifying these phenomena from empirical data depends on something we call accessibility, which refers, roughly, to the degree of separation between the data and the subsystem. The ability to use data to update a model despite limited accessibility is the ultimate goal of model refinement.

In this paper we examine model refinement for a first principles model of the ionosphere and thermosphere. Specifically, our approach is to use the Global Ionosphere Thermosphere Model (GITM) [28] to provide a known initial model.
GITM is a 3-dimensional spherical code that solves the Navier-Stokes equations for the thermosphere. These types of models are more effective than empirical models because they capture the dynamics of the system instead of snapshots of steady-state solutions. GITM is different from most models of the atmosphere in that it solves the full vertical momentum equation instead of assuming that the atmosphere is in hydrostatic equilibrium, where the pressure gradient is balanced by gravity. While this assumption is fine for the majority of the atmosphere, in the auroral zone, where significant energy is dumped into the thermosphere on short time-scales, vertical accelerations often occur. This heating causes strong vertical winds that can significantly lift the atmosphere [29].

The grid structure within GITM is fully parallel and uses a block-based two-dimensional domain decomposition in the horizontal coordinates [30]. Since the number of latitude and longitude blocks can be specified at runtime, the horizontal resolution can easily be modified. GITM has been run on up to 256 processors with a resolution as fine as 0.31° latitude by 2.5° longitude over the entire globe with 50 vertical levels, resulting in a vertical domain from 100 km to roughly 600 km. This flexibility can be used to validate accuracy by running model refinement at various levels of resolution.

First principles models, such as GITM, are drastically influenced by unknowns such as thermal conductivity coefficients and cooling processes in the atmosphere. These effects cannot be directly measured at each altitude. We identify these subsystems, which are assumed to be unknown or uncertain using data that are readily available from simulated satellites on orbit, and we correct the uncertain model to demonstrate the feasibility of implementing model refinement techniques.

2. ADAPTIVE MODEL REFINEMENT FOR SUBSYSTEM IDENTIFICATION

Model refinement is concerned with the identification of a specified subsystem of a larger overall model. The challenge is to perform this identification despite the fact that the subsystem of interest has low accessibility, that is, when neither the inputs nor the outputs of the subsystem are accessible in the form of data. The innovation of this paper is to recognize as in [9, 10, 11, 12, 35] that this problem is equivalent to a problem of adaptive control theory. This equivalence is evident when the model-refinement problem is cast in the form of a block diagram, as in Figure 2.

Figure 2 shows a block diagram of adaptive model refinement. Each block is labeled to denote its uncertainty status. The blocks labeled “Known Subsystem” and “Unknown Subsystem” represent the physical system, whose inputs include known and unknown inputs (also called “physics drivers”). These subsystems are connected through feedback, which captures the fact that each subsystem impacts the other. Although serial and parallel interconnections can also be considered, feedback interconnection provides the greatest generality in practice. The majority of the dynamics of the system are assumed to be included in the “Known Subsystem” block, while the “Unknown Subsystem” block includes static or dynamic maps that are poorly known. The objective is to use data to better understand the “Unknown Subsystem” block.

The lower part of the diagram in Figure 2 constitutes the “Simulated System.” The “Physics Model,” which is implemented in computation, captures the dynamics of the “Known Subsystem” and serves as the initial model. This model is interconnected by feedback with the block labeled “Identified Physics,” which is refined (updated) recursively as data become available. This model refinement occurs through the “Physics Update” procedure, which is denoted by the diagonal arrow. The subsystem model update is a
tuning procedure that recursively identifies the unknown physics to provide a model of the “Unknown Subsystem” block. This tuning procedure is driven by the model-error signal $z$, which is the difference between the data from the “Physical System” and the computed output of the “Simulated System.”

![Block Diagram Illustrating Model Refinement Problem](image)

**Figure 2.** This block diagram illustrates the model refinement problem, where the goal is to identify the “Unknown Subsystem” of the “Physical System.” By depicting this problem as a block diagram, it becomes evident that the model refinement problem is equivalent to a problem of adaptive disturbance rejection.

When cast in the form of a block diagram in Figure 2, the model refinement problem has a form of an adaptive control system. This resemblance suggests that adaptive control methods may be effective in tackling the model refinement problem. To do this, we require techniques for adaptive control that are sufficiently general and computationally tractable to address the features of large-scale physically meaningful applications.

2.1. **Retrospective Cost Optimization.** To address the model refinement problem, we apply techniques that we have developed for adaptive control. These techniques, which are described in [22, 23, 24], are distinct from standard adaptive control approaches in several crucial ways. Specifically, the approach of [22, 23, 24, 35] requires minimal modeling information concerning the “Known Subsystem,” and is applicable to a wide range of adaptive control problems, including command following, disturbance rejection, stabilization, and
model following. The algorithm utilizes a surrogate cost function that entails a closed-form quadratic (and thus convex) optimization step. Surprisingly, the controller update requires information about only the zeros of the system; no information about the poles is needed. Even more surprising is the fact that the control update requires only knowledge of the nonminimum-phase zeros of the system. This result is truly remarkable in that it shows definitively that nonminimum-phase zeros are the crucial modeling information that is needed for adaptive control.

For model refinement, the specific problem of interest is adaptive disturbance rejection, where the “disturbance” to be rejected is the unknown driver \(v\). The performance signal in the example application described below is the error in neutral mass density of the upper atmosphere, and this signal is used to drive the “Physics Update.”

The novel feature of the technique developed in [22, 23] is the use of a 
retrospective cost criterion to update the estimate of the “Unknown Subsystem.” Unlike many adaptive control techniques that are limited to systems with minimum-phase zeros and low relative degree, this approach is effective for systems with arbitrary poles and zeros. This unique flexibility allows us to apply the technique of retrospective cost adaptive control to the problem of model refinement.

Although the techniques developed in [22, 23, 24] apply to linear systems, the example discussed in the next subsection shows that the method can be effective for large-scale nonlinear systems such as GITM. Additional relevant literature on retrospective cost optimization includes [13, 31, 32, 33, 34, 35, 36, 38, 39, 40].

Retrospective cost optimization depends on several parameters that are selected a priori. Specifically, \(n_c\) is the estimated order of the unknown subsystem, \(p \geq 1\) is the data window size, and \(\mu\) is the number of Markov parameters obtained from the known model. The methodology for choosing these parameters is as follows. The subsystem order \(n\), is overestimated, that is \(n_c\) is chosen to be greater than the expected order of the unknown subsystem; for parameter estimation, \(n_c\) is zero. \(\mu\) is generally chosen to be 1, however, a larger value is needed if nonminimum phase zeros are present in the initial model.

The adaptive update law is based on a quadratic cost function, which involves a time-varying weighting parameter \(\alpha(k) > 0\), referred to as the learning rate since it affects the convergence speed of the adaptive control algorithm.

We use an exactly proper time-series controller of order \(n_c\) such that the control \(u(k)\) is given by

\[
(1) \quad u(k) = \sum_{i=1}^{n_c} M_i(k)u(k-i) + \sum_{i=0}^{n_c} N_i(k)y_0(k-i),
\]

where \(M_i \in \mathbb{R}^{l_u \times l_u}, i = 1, \ldots, n_c\), and \(N_i \in \mathbb{R}^{l_u \times l_y}, i = 0, \ldots, n_c\), are given by an adaptive update law. The control can be expressed as

\[
(2) \quad u(k) = \theta(k)\psi(k),
\]

where

\[
\theta(k) \doteq [N_0(k) \cdots N_{n_c}(k) \ M_1(k) \cdots M_{n_c}(k)]
\]
is the controller parameter block matrix and the regressor vector $\psi(k)$ is given by

$$
\psi(k) \triangleq \begin{bmatrix}
y_0(k) \\
y_0(k-n_c) \\
u(k-1) \\
\vdots \\
u(k-n_c)
\end{bmatrix} \in \mathbb{R}^{n_cl_u+(n_c+1)l_y},
$$

For positive integers $p$ and $\mu$, we define the extended performance vector $Z(k)$ and the extended control vector $u(k)$ by

$$
Z(k) \triangleq \begin{bmatrix}
z(k) \\
\vdots \\
z(k-p+1)
\end{bmatrix}, \quad U(k) \triangleq \begin{bmatrix}
u(k) \\
\vdots \\
u(k-p_c+1)
\end{bmatrix},
$$

where $p_c \triangleq \mu + p$.

From (2), it follows that the extended control vector $u(k)$ can be written as

$$
U(k) \triangleq \sum_{i=1}^{p_c} L_i \theta(k-i+1) \psi(k-i+1),
$$

where

$$
L_i \triangleq \begin{bmatrix}
0_{(i-1)l_u \times l_u} \\
I_{l_u} \\
0_{(p_c-i)l_u \times l_u}
\end{bmatrix} \in \mathbb{R}^{p_c l_u \times l_u}.
$$

We define the surrogate performance vector $\hat{Z}(\hat{\theta},k)$ by

$$
\hat{Z}(\hat{\theta},k) \triangleq Z(k) - \hat{B}_{zu} \left( U(k) - \hat{U}(k) \right),
$$

where

$$
\hat{U}(k) \triangleq \sum_{i=1}^{p_c} L_i \hat{\theta} \psi(k-i+1),
$$

and $\hat{\theta} \in \mathbb{R}^{l_u \times [n_cl_u+(n_c+1)l_y]}$ is the surrogate controller parameter block matrix. The block-Toeplitz surrogate control matrix $\hat{B}_{zu}$ is given by

$$
\hat{B}_{zu} \triangleq \begin{bmatrix}
0_{l_z \times l_u} & \cdots & 0_{l_z \times l_u} & H_d & \cdots & H_{\mu} & \cdots & 0_{l_z \times l_u} & \cdots \\
0_{l_z \times l_u} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0_{l_z \times l_u} & \cdots & 0_{l_z \times l_u} & 0_{l_z \times l_u} & \cdots & 0_{l_z \times l_u} & \cdots & \cdots & \cdots \\
\end{bmatrix},
$$

where the relative degree $d$ is the smallest positive integer $i$ such that the $i$th Markov parameter $H_i$ of the initial model is nonzero. The leading zeros in the first row of $\hat{B}_{zu}$ account for the relative degree $d$. The algorithm places no constraints on either the value of $d > 0$ or the rank of $H_d$ or $\hat{B}_{zu}$. 

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We now consider the cost function
\begin{equation}
J(\hat{\theta}, k) \triangleq Z^T(\hat{\theta}, k)R_1(k)Z(\hat{\theta}, k) + \text{tr} \left[ R_2(k) \left( \hat{\theta} - \theta(k) \right)^T R_3(k) \left( \hat{\theta} - \theta(k) \right) \right],
\end{equation}
where \( R_1(k) \triangleq I_p \), \( R_2(k) \triangleq \alpha(k)I_{n_c(l_w^0 + l_w)} \), and \( R_3(k) \triangleq I_{l_w} \). Substituting (3) and (4) into (5), \( J \) is written as the quadratic form
\begin{equation}
J(\hat{\theta}, k) = c(k) + b^T \text{vec} \hat{\theta} + \left( \text{vec} \hat{\theta} \right)^T A(k) \text{vec} \hat{\theta},
\end{equation}
where
\begin{align*}
A(k) &= D^T(k)D(k) + \alpha(k)I, \\
b(k) &= 2D^T(k)f(k) - 2\alpha(k)\text{vec} \theta(k), \\
c(k) &= f(k)^T R_1(k)f(k) + \text{tr} \left[ R_2(k) \theta^T(k)R_3(k)\theta(k) \right],
\end{align*}
where
\begin{align*}
D(k) &\triangleq \sum_{i=1}^{n_c+\mu-1} \psi^T(k - i + 1) \otimes L_i, \\
f(k) &\triangleq Z(k) - \bar{B}_{zz}U(k).
\end{align*}
Since \( A(k) \) is positive definite, \( J(\hat{\theta}, k) \) has the strict global minimizer
\begin{equation}
\hat{\theta} = \frac{1}{2} \text{vec}^{-1}(A(k)^{-1}b(k)).
\end{equation}
The controller gain update law is
\begin{equation}
\theta(k+1) = \hat{\theta}.
\end{equation}
The coefficients of the time series (1) contain information about the unknown subsystem. For parameter estimation, the entries of \( \theta(k) \), in the case \( n_c = 0 \), are parameter estimates that can be used to correct the initial model. For dynamic subsystem identification, the entries of \( \theta(k) \), when \( n_c > 0 \), are parameters of a system of equations that describe the unknown dynamics. We demonstrate the both scenarios on GITM.

3. Application of Model Refinement to Ionospheric Parameter Estimation

To illustrate adaptive model refinement, we consider the problem of using upper atmospheric mass-density measurements, as can be obtained from a satellite, to estimate the thermal conductivity of the thermosphere. This problem is challenging due to the fact that we do not assume the availability of measurements that can serve as inputs or outputs to the “Unknown Subsystem” modeling thermal conductivity. In other words, the objective of the identification in this particular application is inaccessible relative to the available measurements. Furthermore, the identified subsystem parameters must be physically representative of the unknown subsystem. Specifically, the identified subsystem must not only refine the true model such that the closed-loop outputs of the known and unknown subsystem match the output of the known and identified subsystem, but the identified parameters must also match the unknown parameters to provide useful information about the unknown physics of the system.
Figure 3. This block diagram specializes Figure 2 to the case of model refinement for a model of the ionosphere-thermosphere. Simulated data are generated by using the 1D Global Ionosphere-Thermosphere Model (GITM), where the thermal conductivity is assumed to be unknown. The goal is to estimate the thermal conductivity by using measurements of the neutral mass density. The fact that this problem is precisely a problem of adaptive control allows us to apply retrospective cost adaptive control methods. This problem is difficult for conventional parameter estimation methods due to the low accessibility of the unknown physics relative to the available measurements.

We use GITM to simulate the chemistry and fluid dynamics in a 1D column in the ionosphere-thermosphere. The temperature structure of the thermosphere depends on many factors, such as the Sun’s intensity in extreme ultraviolet (EUV) wavelengths, eddy diffusion in the lower thermosphere, radiative cooling of the O$_2$ and NO, frictional heating, and the thermal conductivity.

The basic structure of the thermal conductivity is $\lambda = AT^s$, where $A$ and $s$ are the thermal conductivity and rate coefficients, respectively. The thermal conductivity may depend on chemical constituents (e.g., N$_2$, O$_2$, and O). Uncertainty concerning the values for $A$ and $s$ [27], can strongly control the temperature structure. The need to estimate these coefficients from available data is shown in Figure 4, where published values of these coefficients vary depending on the reference source. We use this uncertainty in the literature as a bound on performance. Ideally, the estimates we obtain using data should be within these bounds.
To estimate the unknown thermal conductivity coefficient, we apply the retrospective cost adaptive control algorithm to the simulated measurements of neutral mass density provided by 1D GITM. We do this by running a “truth model,” from which we extract mass-density data at 400-km altitude (a typical altitude for satellites). The thermal conductivity coefficient is initialized to be zero, and its value is updated recursively by the retrospective cost adaptive control algorithm. Figure 5 shows the evolution of the estimate of the thermal conductivity as more data become available. The estimate is seen to converge to a neighborhood of the true value within about $0.6 \times 10^4$ data points.

To further illustrate the model refinement method, we now assume that both the thermal conductivity, $A$, and rate coefficient, $s$, are unknown. The parameters $A$ and $s$ are initialized as zero, and are updated simultaneously and recursively. Figure 6 shows the update of the estimates. Both estimates converge to within a neighborhood of the true values within $0.6 \times 10^5$ data points.

The performance gains attributed to the refined parameters are shown in Figure 7. The upper figure is a performance comparison of a nominal GITM model, which is assumed to be the truth model, while another GITM model with a thermal conductivity coefficient is set to zero. Within the simulated model, this value prevents energy deposited in one layer of the atmosphere from remaining in that layer. The lower plot of Figure 7 illustrates the reduction in model error obtained by including the identified coefficients, thereby accounting for the thermal conductivity of this species. The benefits of refining the GITM model are evident by the improvement in model accuracy.

4. Application of Model Refinement to Ionospheric Dynamics Estimation

To illustrate model refinement in the case of an unknown dynamic subsystem, the NO radiative cooling was removed from GITM to provide an initial model but retained in GITM for the truth model. The goal is to reproduce the missing process. This is nontrivial since the functional form of the cooling was assumed to be unknown as were the dynamics. We assumed only that something was missing from the energy equation, and that this was most likely a function of temperature. The dynamics of the cooling were estimated at
Figure 5. This plot shows the true and estimated thermal conductivity coefficient. The initial guess for the thermal conductivity is zero. The estimate converges to a neighborhood of the true value within about $0.6 \times 10^5$ data points. The lack of final convergence is due to nonlinearities in the dynamics of the system. However, the oscillations are well within the uncertainty bounds, which reflect the range of published values for this coefficient.

Three different altitudes, connecting the other altitudes through linear interpolation, which is obviously an approximation, but illustrates the technique. Nothing else about this energy sink was assumed. The thermospheric density was utilized as data at 407 km altitude from a simulated truth model that included NO cooling. The result of the model refinement in Figures 8 and 9 demonstrates that this technique captured the actual dynamics in the system. The height profile of the cooling matches the actual cooling quite well. Furthermore, the temporal variation of the maximum cooling matched the cooling simulated by the model.

Three linear dynamical equations were derived (one for each of the three chosen altitudes), which reproduced the dynamics of the cooling. To determine the relevant drivers, the temperature estimate was fed into the model refinement technique. What resulted was a profile that looks remarkably like the natural logarithm of the NO density, indicating that this may be the source of the cooling, which it actually is. This technique can thus be used to refine and improve an initial model (or models, if several are hypothesized) that is either uncertain or erroneous. In turn, the improved model provides a more accurate foundation for data assimilation aimed at wind and density estimates in the presence of solar storm disturbances. Figure 10 shows a comparison of the model without correction versus the model with correction, both of which are baselined against the truth model. Without data-based model refinement, the estimated density measurements degrade as time increases.
Figure 6. These plots show the true and estimated thermal conductivity coefficient as well as the true and estimated rate coefficient. The initial guesses for both coefficients are zero. The estimates converge to a neighborhood of the true value within about $0.6 \times 10^5$ data points. The estimates are also within the uncertainty limits, which are determined by the range of published values for these coefficients.

5. Conclusions

In this paper we presented a method for improving the fidelity of models using empirical data, which is known as model refinement. Model refinement presents challenges relative to standard input-output system identification, specifically, a lack of accessibility to the signals required to identify the refining subsystem. For model refinement we use retrospective cost optimization to identify the unknown model. We demonstrated the feasibility of the method in refining first principles models. In particular, to model the ionosphere and thermosphere using the global ionosphere-thermosphere model (GITM). We demonstrated how uncertain parameters are identified when the structure of the refining model is known. Furthermore, we demonstrated how unknown dynamics are identified from data when the internal structure of the updated subsystem is unknown.

References

Figure 7. The upper figure shows the difference in neutral mass density output between the truth model and the initial model. The lower figure shows the difference in neutral mass density output between the truth model and the refined model. By utilizing empirically refined estimates of the thermal conductivity and rate coefficient, the model error is reduced.

Figure 8. This plot shows the difference between the actual NO cooling included in the truth model and the cooling estimated by the model-refinement technique as a function of time at a specific altitude (152 km). The vertical dashed lines are the time instances when the altitude vs. NO cooling plots in Figure 9 are taken.

Figure 9. These plots show the difference between the actual NO cooling included in the truth model and the cooling estimated by the model-refinement technique as a function of altitude at a given time. Cooling is along the horizontal axis, while altitude is along the vertical axis. The blue dashed line is the estimated value. The measured data were taken at an altitude of 407 km. The vertical dashed lines in Figure 8 are the time instances when the altitude vs. NO cooling plots are taken.


FIGURE 10. This plot shows the difference between the density measurements for the initial model, where no correction is made, and the model with the refined subsystem versus the truth model. We note that, with model refinement, the refined model is able to track the truth model, whereas, in the case that no correction is made, the density measurements degrade as time increases.