Abstract

Global gyrokinetic models have been shown to accurately predict the ion conduction, χ_i, by incorporating microturbulence into the models. Extreme-scale, fixed-flux supercomputing simulations are beginning to simulate modes of operation relevant to next-generation(ITER,DEMO) reactors. Using a surrogate model to reduce the computational expense of XGC simulations, I conduct a predictive scan in ρ^{-1} , to ascertain whether or not the ion diffusivity χ_i scales in a Bohm or gyro-Bohm fashion, and analyze the sensitivity of χ_i to perturbation in the heating model.

Predicting the Scaling Relationship Between Ion Heat Conduction and Plasma Reactor Size Under Uncertainty Using Surrogate Models

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Contents

1 Introduction

1.1 Magnetically Confined Fusion

The history of nuclear fusion research dates to the 1920's, when Arthur Eddington suggested in his book "The Internal Constitution of Stars" that the transmutation of hydrogen atoms through nuclear fusion into helium is responsible for powering the energy released by the sun.[1]. In 1934, Ernest Rutherford and his assistant Mark Oliphant successfully fused deuterium by generating voltages of 400,000V, colliding deuterium atoms with deuterium atoms. They reported a net release of binding energy of $4MeV$ per $D - D$ reaction, making it an energetically favorable.[2]. In his 1939 article, "Energy Production in Stars",[3] Hans Bethe posited that only 2 elements lighter than carbon were stable for a long enough period to provide a fuel source for the nuclear fusion reactions that take place in faint stars: H^2 and He^4. He^4 is in fact too stable an element to be a solar fuel source, indicating that the nuclear reactions in stars could only be explained by a

$$H^2 - H^2 \rightarrow He^3 + n$$
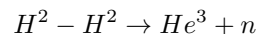
reaction.

Research dedicated to producing and controlling nuclear fusion reactions, as a method of power and energy production, led to the U.S., Russia, France and Japan building fusion reactors in the 1950s. In 1958 Russian scientists built the first tokamak fusion reactor, a toroid shaped reactor which is the Russian translation of "Toroidal Chamber with Magnetic Coils." The toroidal design is the standard in fusion reactor design as the toroidal shape is ideally suited to the magnetic fields required to confine a plasma. Please see the first figure for a tokamak design image. Today, international research and development support from over 30-member countries is being dedicated to the tokamak International Thermonuclear Experimental Reactor (ITER), which is being built in Cadarache, France. ITER is a full-scale experimental reactor that is the last step before building a demonstrative reactor (DEMO), with the goal of developing a full theory of plasma within an ITER

scale fusion reactor and solving all the engineering problems related a working fusion reactor.

Current fusion research focuses on the deuterium-tritium fusions reaction [4], given by

$$H^2 + H^3 \rightarrow \alpha + n + 17.6 MeV$$
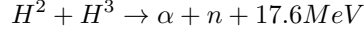
as it is more energetically favorable than the $D - D$ reaction by an order of 14 MeV per reaction.

When deuterium and tritium fuse, an α particle, or He^4 particle is released, as well neutron are

released. $14.1 MeV$ of the released binding energy is transferred to the neutron in the form of kinetic

energy, with $3.5 MeV$ transferred to the α particle.

To generate nuclear fusion reactions deuterium-tritium fuel is placed into a suitable reactor. The

reactor provides initial heating power to start the begin the nuclear fusion process. In an ideal

system there is a critical plasma temperature that, once reached, implies that the α particles have

enough energy to sustain the nuclear fusion reactions in a steady, allowing the initial heating source

to be turned off.

Countering the heat produced by the α particles are the heat transport processes; thus, a realistic

operating temperature must account for the heat lost due to these heat transport mechanisms.

The sources of heat or energy loss inside a plasma include Bremsstrahlung radiation, or charge

acceleration resulting in radiation, diffusion through Coulombic interactions, and ion heat transport

through micro-turbulence. In equation form, the balance of power between the α particle heating

and all the above heat sinks is given by

$$S_\alpha = S_B + \chi \frac{\partial T}{\partial r}$$

Where S_α is the α heating power, S_B is the power lost by Bremsstrahlung radiation, and $\chi \frac{\partial T}{\partial r}$

account for the heat transport out of the plasma, and χ is a general heat transport coefficient.

Since most of heat transport happens through ion heat conduction, I will refer to χ as the ion heat

transport coefficient from now on.

This balance is referred to as power balance in a plasma and must be met for the fusion reactions

in a plasma reactor to become self-sustaining. This balance is dependent on three important reactor characteristics: the internal pressure generated by the magnetic fields, p, the confinement time of the plasma, τ and the temperature of the plasma. The minimum $\{p\tau, T\}$ pair is given by $\{p\tau, T\} = \{8.3atm\ s, 15keV\}$

1.2 Diffusion, Neoclassical Theory, and Scaling Laws

There are 2 primary mechanisms that contribute to ion heat conduction out of the plasma. The first is neo-classical transport, which is classic transport caused by Coulombic interactions applied in a toroidal geometry, where the Coulombic collisions occur as the ions traverse along their polar orbit. Plasma heat conduction is considered to have been one of, if not the most, difficult challenges on the way to building a working reactor. This is because ion heat conduction is driven by plasma micro-turbulence, as such a full theory and model of heat transport must include micro-scale turbulent physics. This turbulence is driven by severe ionic thermal gradients, resulting in fluctuations in the electric and magnetic field that perturb the guiding center orbits of the ions about the magnetic field lines. This randomness in fluctuations leads to collision like diffusion in particles and energy [4], and accounts for most of the diffusion. The models required to accurately simulate micro-turbulence are kinetic, requiring computationally expensive direct numerical simulations .

One of the primary methods for understanding the relationship between current plasma reactor research data and future reactor performance is to use scaling relationships. If two systems are geometrically similar or dynamically similar, scaling relationships between the systems by dimensionalizing the system parameters, and scaling these parameters to the relevant size. For example, if a small wind tunnel system comprised of an airfoil with an airflow over its surface has identical geometric ratios to a full-size airfoil, and the dynamics of the flows over the flows are similar, then a scaling relationship between the boundary layer height can be made between the two systems.

In the case of the ITER reactor, the scaling law of interest is the scaling relationship between the dimensionless reactor size, which is given by the dimensionless ratio $\rho^* = \rho_i/a$, and the ion heat conduction χ_i. The power output of the nuclear fusion reactor is implicitly contained with the dimensionless radius.

Predicting how heat conduction scales with reactor size is critical to designing and building ITER scale reactors, as the required input heating must be understood to maintain power balance in ITER reactor. Current research [5] have used full-function simulations, which include plasma micro-turbulence and collision phenomenon, to predict the scaling relationship between ρ^* and χ_i. The results of this study predicted a linear scaling relationship, which is undesirable, as this indicates that required heat input to maintain plasma temperature scales linearly with reactor size. This study was not complete, as the simulation as run on 1/6 of the full reactor size, with periodic boundary conditions implemented to generate a full reactor. This leave the possibility for missing EM modes that are larger than 1/6 the size of the reactor. This research can be further developed by running a simulation on the full reactor to capture these missing modes, which is a part of the work that will be completed in this thesis.

1.3   Gyrokinetic Equations, XGC Code, and Heating Model

The mathematical model of the for a tokamak plasma is the 5-D gyrokinetic model, which is the Boltzmann equation with the Lorentz force substituted into the acceleration term, also known as

the Vlasov-Boltzmann equation [6]. This model includes Maxwell's equations.

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + e(E + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{v}} = C(f) + Source + Sink$$

$$\nabla \cdot \mathbf{E_0} = \frac{\rho_c}{\epsilon_0}$$

$$\nabla \cdot \mathbf{B}_0 = 0$$

$$\nabla \times \mathbf{E}_0 = -\frac{\partial \mathbf{B}_0}{\partial t}$$

$$\nabla \times \mathbf{B} = \frac{j}{\epsilon_0 c^2} + \frac{1}{c^2}\frac{\partial E_0}{\partial t}$$

The first term of the Vlasov-Boltzmann equation is the changing particle density as a function of time, the second term is the momentum transport term, and the second term is the energy transport term. C(f) is the collision operator, which includes the micro-turbulence fluctuations, and the sink includes the ionic heat diffusion out of the system. The rest of the equations are Maxwell's equations. To implement this model, including the multiscale collision and turbulent physics, the XGC code was developed by the Center for High-Fidelity Boundary Simulation. This code can capture full-function multiscale physics and is the simulation that was used in previous research to determine the relationship between ρ^* and χ_i. The XGC code is a first principle, kinetic model, particle in cell code that takes in a particle location vector, and results in a particle and velocity distribution based on the physical constraints. The XGC simulation includes a heating model component that takes the position distribution and velocities of the particles from the XGC results, and translates these outputs into the ion heat diffusivity through the following equations [7]

$$T_i = \frac{1}{3} \sum_{x_j \in \Delta V} w_j m_i (2B\mu + (v_{||j} - u_{||})^2)/W$$

$$q_{i\Psi N} = \frac{1}{2} \sum_{X_j \in \Delta V} m_i (2B\mu + (v_{||j} - u_{||})^2)\dot{\mathbf{X}} \cdot \nabla\Psi/W$$

$$\chi_i = q_{i\psi}/(|\nabla|^2 \frac{\partial T}{\partial \Psi}).$$

Where ΔV is the volume, Ψ is the spatial domain, m_i, $q_{i\Psi}$, and χ_i are the particle masses, heat flux in Ψ space, and chi_i is the thermal conductivity of the ions. w_i and W are individual weights and

the sums of these weights, $\dot{\mathbf{X}}$ is a vector of the particle velocities, $v_{||j}, u_{||}$ are the velocities that are parallel to the magnetic fields, and the average of these velocities, respectively. Thus, the diffusion coefficient is solved for.

While the XGC code is a full-f simulation, and is self-consistent, it is computationally expensive, requiring 15,000-25,000 CPUs to run simulations for $DIII - D$ scales experimental reactors. ITER simulations require extreme scale computing at the level of Titan, Edison and, Mira, and even at these scales requires a full day to complete one simulation. Characterizing uncertainty in χ_i requires multiple simulation runs with data under uncertainty to propagate uncertainty through the model. To reduce the computational expense characterizing χ_i I propose the development of a surrogate heating model that is trained on the output of limited, already performed runs from the full-f simulation. The full details on the experimental methodology to be used can be found in the following section.

To reiterate the stated outcome of this thesis, the primary goal of this thesis is to computationally develop the scaling relationship between ionic heat conduction, χ_i, and the dimensionless reactor size $\rho^* = \rho_i/a$ by developing a surrogate model that is trained on the outputs of the full-f XGC model.

2   Experimental Methodology

Prediction under uncertainty is often an expensive and complicated process[8, 9]. The tradeoff between the computational cost of complex models and the loss of predictive accuracy associated with simpler models may be addressed by emerging multifidelity UQ approaches[10, 11].

In magnetic confinement fusion, there is an important, clearly defined set of prediction scenarios, corresponding to modelling future reactor(ITER/DEMO) performance. Even a "high-fidelity", extreme-scale model such as XGC, still has a parameter space of large enough dimension to make a

brute-force, sampling-based predictive process impossible. The traditional approach to prediction, with or without extrapolation, is to sample the model parameter input space $\theta = \theta_1, \theta_2, \ldots, \theta_d$, evaluate the model, and return a quantity of interest (QoI) $Q(\theta)$. Most realistic QoI maps are nonlinear in the QoI map(even if the governing PDE is linear), so the probability distribution function(PDF) of $Q(\theta)$ will have to be estimate in a non-parametric way, typically by kernel density estimation, or by computing empirical statistics from samples. The mean-integrated squared error of the approximate PDF converges with a rate of $\mathcal{O}(N^{-2/(d+4)})$, where N is the number of samples of the model and d is the dimension of the input space. As each sample typically involves a PDE solve and subsequent post-processing, this process quickly becomes exorbitantly expensive.

2.1 Surrogate Models

A surrogate model replaces the large cost of the model solve with a fast, explicit function evaluation. The surrogate model is constructed via interpolation or regression on a modest number of potentially deterministic traning samples M. The error from insufficient samples in the kernel density estimation is exchanged for the error between the true QoI $Q(\theta)$ and surrogate QoI $Q_S(\theta)$[12]. Sparse grid approaches [13, 14] give roughly the same error(modulo a factor of n^{d-1}, where d is the dimension of the (input) parameter space and n is the number of training points)) as traditional tensor-product surrogates. However, the number of samples is $\mathcal{O}(2^n n^{d-1})$, instead of the full grid cost of $\mathcal{O}(2^{nd})$. These savings and accuracy can potentailly be increased by adopting adaptive sparse grid surrogates[13].

Augmented Surrogates

In predictive extrapolation, the target scenario for $Q(\theta)$ is often sufficiently expensive to even make the surrogate approach tenuous. One strategy in this situation is to construct the surrogate using a sequence of lower-fidelity models to construct $\tilde{Q}(\theta)$, and then train the surrogate[11]. This often requires a good characterization of the error between $Q(\theta)$ and $\tilde{Q}(\theta)$. This is not a well-explored or

understood area in the kinetic plasma PIC community.

Another approach is to add deterministic parameters that describes "nearby" scenarios, s.t. $Q(\theta) = A(\theta, k_1, k_2, \ldots, k_r)$, k_i fixed. We call the determanistic parameters k_i augmentation parameters, and the surrogate model A_S of A, the augmented surrogate. Moderate gains are achieved when the number of augmentation parameters is small and the cost of sampling A outside of the prediction scenario Q is much cheaper. If the gradient of A with respect to θ is only weakly dependent on the augmentation parameters, significant (cost-based) accuracy savings can be achieved.

There are two fundmental assumptions in the construction of an augmented surrogate of a n-dimensional predictive scenario $Q(\theta_1, \theta_2, \ldots, \theta_n)$.

1. There exists small number m of (usually deterministic) parameters $d_1, d_2, \ldots, d_m$ that characterize nearby n-dimensional predictive scenarios $\tilde{Q}_i(\theta_1, \theta_2, \ldots, \theta_n)$.

2. The cost of a sample from the nearby scenario, $C_{\tilde{Q}_i}$, is much less than the cost C_Q of a sample from the desired prediction scenario.

The *augmented surrogate* is a surrogate model $A(\theta, d)$ constructed on training data $\{(\theta, d), \hat{Q}(\theta, d)\}$ in the $m + n$-dimensional parameter space.

Adaptive sparse grid method

The classical sparse grid method is dimension agnostic[13]. All interactions of the same order are treated equally. Often, a small subset of variables and interactions contributes significantly to the variability of the function $Q(\theta, d)$. If the variability in the θ-dimensions is greater than the variability in the scenario parameters($\{d_i\}$) then the overall cost of constructing the larger dimensional surrogate is actually less, due to the cheaper computational cost of $\tilde{Q}_i$.

We modify the greedy algorithm for constructing h-adaptive generalized sparse grid (h-GSG) in [14]. The hierarchical surpluses for the current sparse grid are modified with a cost weight $W_C(d_1, d_2, \ldots, d_m)$ that approximates the relative cost of simulating the added sparse grid point,

and a m-dimensional distance metric that penalizes sparse grid samples that are too far away from the prediction scenario $Q(\theta)$. This encourages parameter exploration in θ_i-dimensions at inexpensive simulation levels, while rewarding coarse grid points that reduce the local surrogate error near the prediction scenario $Q(\theta)$.

2.2   Proposed UQ Study

We will conduct a base parameter scan in (ρ_*), at the mean values of the uncertain inputs. This will verify that wedge, Eulerian versus PIC, or other factors do not impact the conclusions reached in [5]. This scan will also provide the first training runs for the augmented surrogate A.

Data from a range of ρ_*^{-1} simulations in the interval (100,600) will be provided by Varis Carey and other members of the HBPS Scidac team from supercomputer simulations run at NERSC and Oak Ridge facilites. A budget of 20,000 SU at NERSC has been allocated for providing the data for this scaling study(which is already partially complete at the time of this proposal) and for additional simulations to train the augmented surrogate to cover the input parameter space. The main input parameters parameterize the location, slope, and shape of the core heat source and boundary sink. Additional parameters covering torque will be allowed if the computational budget allows further investigation. If NERSC resources are expended, certain (small-scale) simulations will be conducted on CU-Denver or RMCC resources(Summit) under the supervision of Varis Carey.

Postprocessing Software

Postprocessing software (python and Matlab) are available to extract plasma QoI from XGC 2D and 1D diagnostic output. The BPS team will arrange a NERSC account for Evan to avoid transfer of large binary files and allow simulation data to be repurposed for serving the plasma fusion community.

2.3 Contingency Research Plan

Large scale gyrokinetic simulations, especially at large values of ρ_*^{-1}, involve considerable resources, and certain stability requirements for the simulations are only roughly known *a priori*. In the event of insufficient data to build the ρ_* augmented surrogate, we will instead switch to looking at the effect on transport of uncertanties in the background magnetic field. This is actually a harder problem as the perturbations (i.e. the samples) must be valid solutions of the Grad-Shrafanov equations. We will investigate this in a 1D or 2D slab geometry using standard techniques uncertainty quantification techniques. This will also be a publishable, impactful result, and could affect future work in 2D(axisymmetric) or 3D tokamak geometries.

3 Literature Review for MIS Thesis Proposal

Determining the plasma size scaling of the ion diffusivity, and performing efficient sensitivity analysis on the ion diffusivity in the heating component of the XCG model, within a constructed surrogate model, will require a knowledge base in the following subjects.

Plasma Physics, Gyrokinetic Plasma Models, & Plasma Simulation

To perform this research, a knowledge base in plasma physics, current research in ITG driven turbulent transport, and nuclear fusion modeling and simulation methods must be developed. To assist in developing this knowledge base I have identified the following references.

Jeffrey P. Friedberg Plasma Physics and Fusion Energy [4]
> This textbook covers the physics of plasma fusion, its applications as an energy sources, the physical requirements to create an energy producing fusion reactor, and the designs requirements for fusion reactor with a toroidal geometry - the geometry of the ITER fusion reactor.

Characterizing the turbulence driven ion heat transport is active research as, per Idomura, "it is of critical importance in predicting performances of future fusion devices, which will be several times larger than the present experiments." [5] Thus, the following articles, with pertinent findings, are reviewed for information relevant to this thesis proposal.

Improving gyrokinetic models, and increasing computational power, has led to iterative improvements in simulating the ion temperature gradient (ITG) driven turbulence, and heat transport. In Ref [15] Y. Idomura implemented a full-f gyrokinetic Eulerian GT5D Vlasov simulation, including sources and collisions to study ITG driven turbulence heat transport. In Ref [16] Y. Idomura used the same full-f GT5D simulation to explore the scaling relationship between χ_i and ρ^* for values of $\rho^* = \frac{1}{100} - \frac{1}{225}$ by increasing the radius of the cross-sectional area of the tokamak reactor, a, and by increasing the plasma input power. Simulation results showed that intrinsic momentum parallel to the magnetic field damps out transport phenomenon. With intrinsic momentum built up, the transport was shown to scale sub linearly with ρ^*, while without intrinsic momentum global transport scales linearly with ρ^*. with the resulting heat conduction scaling transitioning from linear, or Bohm like, to sub-linear, or gyro-Bohm like, as reactor size increased .

In Ref [5] the above scan is performed, with the plasma power explicitly scaled with increasing plasma size for ρ^* and power value pairs were $\rho^*, P = [150, 4MW, 300, 8MW, 450, 12MW, 600, 16MW]$. S. Ku et al have released a very interesting full-f paper on ITG turbulence.

Plasma Modeling Methods and Applications - Textbook [6]

This is a modern textbook that covers kinetic theory plasma models, fluid equations and hybrid plasma models, and applications of these models. Each model is developed from first principles, making this an invaluable source for understanding the 5-D gyrokinetic model, as well as a reliable source for the developing and implementing the models that were discussed

in the educational section of this proposal.

"Plasma Physics via Computer Simulation" - C K Birdsall, A B Langdon [17] This is a classic text on plasma modeling and computer simulation and will be useful as an additional reference for the modeling aspect of this thesis. Dr. Wei-Lee from the Princeton Plasma Fusion Physics Laboratory has posted the lecture notes and homework assignments from a course on Theory and Modeling of Kinetic Plasmas on his website.

http://w3.pppl.gov/ wwlee/

This course contains the background information on gyrokinetic model that is being used to describe the plasma boundary physics in the ITER Tokamak reactor.

Project Description

The project proposal from the Partnership Center for High-Fidelity Boundary Plasma Simulation provides the motivation for performing this research, as well as a reference list containing relevant literature that will be reviewed and cited as necessary.

XCG User Handbook - This online handbook provides preliminary information to understand how to use the XCG simulation software. There is contact information available to constant managing code users/developers.

Scaling Relationship Between Ion Heat Diffusivity, χ_i, and Dimensionless Radius $\rho* = \rho_i/a$

Two articles are cited in the literature when referring to scaling arguments between plasma ion heat diffusion and $\rho*$. Both articles provide a lot of clarity to the nature of the scaling parameters that are affiliated with heat diffusion.

Non-Dimensional scaling of turbulence characteristics and turbulent diffusivity - G.R. McGee et al.[18]

Gyro-radius Scaling of Electron and Ion Transport - C.C. Petty et al [19]

Mathematical Analysis

The mathematical component of my degree will be fulfilled through applications of numerical methods in accurate PDE model simulation, uncertainty quantification, surrogate model construction, and exact model validation.

Uncertainty Quantification

Ralph C. Smith - Uncertainty Quantification [20]

Ralph C. Smith has written an introductory textbook on uncertainty quantification that provides useful models, examples and problems to guide the educational and experimental components of this thesis. The textbook has all the background knowledge necessary to develop a toy surrogate model as proposed in this document.

Machine Learning "Gaussian Processes for Machine Learning" - Rasmussen and Williams. [21]

A textbook on machine learning will be useful when developing the surrogate model for this experiment.

Case Study to Understand Current Methods in Uncertainty Quantification

I am currently reviewing a paper referenced from the project proposal titled Improved profile fitting and quantification of uncertainty in experimental measurements of impurity transport coefficients using Gaussian process regression by Chilenski et al. to develop an understanding of the uncertainty quantification and parameter estimation pipeline.[22]

General Probability and Statistics

Performing this work requires a base understanding in probability, Bayesian statistics, and data reduction and error analysis. The following textbooks have been identified to provide a base level of understanding of these topics.

Data Reduction and Error Analysis for the Physical Sciences - Philip R. Bevington, D. Keith Robinson - This textbook contains introductory methodology in data reduction, error analysis, probability, and statistics, with plenty of useful examples.

Data Analysis - A Bayesian Tutorial by D.S. Sivia - This is an introductory textbook in Bayesian statistics, which will be employed throughout this project.

Textbooks

1. Plasma Physics and Fusion Energy by Jeffrey Friedberg

2. Plasma Modeling Methods and Applications

3. Uncertainty Quantification: Theory, Implementation, and Applications by Ralph C. Smith

4. Data Analysis - A Bayesian Tutorial by D.S. Sivia

5. Data Reduction and Error Analysis for the Physical Sciences by Phillip R. Bevington and D. Keith Robinson

Articles

4 Educational Exercises

To familiarize myself with the above experimental methods, I propose the following framework constructed of setting up a toy problem and implementing said toy problem. First numerically evaluating

a familiar PDE model using a finite difference method- possibly the 1-D diffusion equation or the 1-D neutron transport equation - then propagating the uncertainty of the parameters through the model to develop a distribution of the quantity of interest. The neutron diffusion model is appealing as there are libraries available on the distribution of the nuclear cross-section that can be used for uncertainty quantification [20].

After creating a backbox to generate the quantity of interest under uncertainty, I can then use these generated quantities along with the available inputs to construct a surrogate model using methods of linear or nonlinear regression. The quadratic response surface model has been identified as a surrogate modeling method to perform this task. After constructing said surrogate model, the approximate quantity of interest can be compared to the quantity of interest of the real model, with statistics and correlations run on the QoI's. The surrogate models will be run under uncertainty as well, with a statistical comparison run on QoI distribution. To achieve a more accurate surrogate model, I will update the surrogate model based on the QoI distribution.

The understand the complexity associated with scaling into N-D, as we will in this project, the finite difference model will progressively be scaled from 1-D to N-D. The above framework for uncertainty quantification and surrogate model creation and evaluation will be performed as the dimensionality of the system is increased. My thesis will contain all this information as a guiding example for the actual research being performed.

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