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Abstract

Ion diffusion at ITER scales must beGlobal gyrokinetic models have been shown to accurately predict the ion diffusivity by incorporating microturbulence into the models, χ_i. 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.

Integrated Science Thesis Proposal

Evan Shapiro

Master's of Integrated Science, University of Colorado Denver

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1 Introduction

1.1 Magnetically Confined Fusion

The history of nuclear fusion research dates back 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.In 1934, Ernest Rutherfor and his assistant Mark Oliphant succesfully fused deuterium by generating voltages of 400,000V, colliding deuterium atoms with duterium atoms. They reported a net release of binding energy of $4MeV$ per $D-D$ reaction, making it an energetically favorable.In his 1939 article, "Energy Production in Stars", Hans Bethe posited that only 2 elements lighter than carbon were stable for a long enough period of time 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 reactos 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.

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

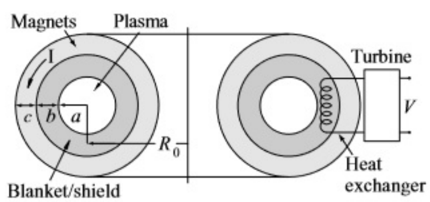
$$H^2 + H^3 \rightarrow \alpha + n + 17.6MeV$$

as it is more energetically favorable than the $D-D$ reaction by an order of 14 MeV per reaction. When detuterium and tritium fuse an α particle, or He^4 particle, and a neutron are released. $14.1 MeV$ of the released binding energy is given to the neutron in the form of kinetic energy, and the remaining given to the α particle. It can be shown that the operating temperatures of a fusion reactor starts at around 10KeV, which is well above the ionizing temperature of hyrdogen and helium, leading to deuterium-tritium fuel to becoming a plasma within a fusion reactor.

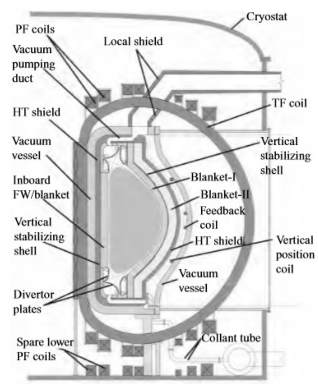
Fusion reactor design uses the energy of the α particle for maintaining the temperature of the plasma, while the energy of the neutron, which is allowed to escape the plasma into the blanket of the reactor, is responsible for heating and powering a stems turbine. For a fusion reactor to be viable as a power source, it must be take an initial heating input to develop a deuterium-tritium fuel source into a self sustaining plasma. Self sustaining means that the α heating is able to balance the heat losses due to Bremsstrahlung radiation, neutron espace, and ion diffusion out of the system.This balance is called the principal of power balance; it cannot be emphasized enough that meeting and maintaining power balance within a fusion reactor is critical to fusion power becoming a viable energy source.

One of the chief concerns in fusion reactor design is heat diffusing out of the magnetically confined region by way of ions, also referred to as ion heat diffusion. Ion heat diffusion is responsible for the majority of the heat lost by the plasma, and as such much attention has been paid to the mechanisms causing this heat loss. To illustrate the principal power balance let us look at 0-D conservation of energy equation for fluids. This equation is given by

The plasma is contained within the inner cylinder of a toroid, with the first wall of the cylinder being protected by a strong magnetic field that shields the wall from thermal loading from the $14.1 MeV$ neutrons, Bremsstrahlung heat loss, and heat conduction. Inside the first wall is the region called the blanket and shield, which is the region of heat exchange for powering an external steam turbine, and provides a tritium breeding ground that sustains the supply of tritium required for the fusion reaction. Outside of this region is the a shield wall which prevents the escape of any radioactive neutrons or gamma particles. The final layer of the toroid contains the superconducting toroidal solenoid, which generates the $10 - 15[T]$ magnetic field inside of the fusion reactor, which again is responsible for confining the ionic and electron components of the plasma inside the reactor. Figures 1 shows the generic theoretical cross-sectional area of toroidal reactor, while figure 2 shows the cross-sectional area of the ARIES-AT tokamak design.



(a) Generic toroidal fusion reactor showing the plasma, blanket-and-shield, and magnets. Image Source J. Friedberg [1]



(b) Cross section of the ARIES-AT power core conguration (courtesy of F. Najmabadi). [1]

Not shown in the picture is the center, or donut hole, of the toroidal reactor. In current reactors, there is an additional magnet in this region that produces a poloidal magnetic field, which when combined with the toroidal magnetic fields produces the magnetic field lines, as seen in figure 3. Due to the Lorentz force, this configuration of magnetic field lines manages to capture the majority of the diffusing ions and electrons in a helical tractory around the magnetic fields lines due to to the Lorentz force on the charged particles.

1.2 Diffusion, Neoclassical Theory, and Scaling Laws

Let's analyze this equation: The first term accounts for the variation of energy flowing into and out of the system with respect to time, the second term accounts for energy lost or gained due to convection of heat out of the system, the third term accounts for energy losses due to compression and expansion of the plasma within a reactor, the 4th term account for heat losses due to diffusion and conduction, and S accounts for the sources and sinks available to the plasma. The sources are the α particle heating due to the D-T nuclear reaction and any auxiiliary heating being supplied to the plasma, while the sinks are the neutrons escaping the plasma into the blanket surrounding the reactor, and Bremsstrahlung radiation.

Assuming that the power production in the reactor has reached a steady state the time term drops out, as well as the convection and compression terms, leaving the 0-D energy conservation equation:

$$\nabla \cdot \vec{q} = S.$$

This equation makes intuitive sense. In equillibrium, if the diffusive processes are matched by the power sources sources and sinks, then a power balance will be achieved in the equation. If the diffusion of heat out of the system increases, α particle heating has to increase to maintain power balance in the reactor, decreasing the efficiency of the reactor.

Maintaining a plasma reactor with a viable power output requires that the transport of heat out of the plasma be balanced by the alpha heating power of the plasma. Characterizing the heat conduction parameter, or ion heat diffusivity χ_i, in a plasma is current research, [2] [3] as it is the primary heat loss mechanism in a tokamak reactor. Per Friedberg In a plasma there are three important types of transport: heat conduction, particle diffusion, and magnetic eld diffusion. Of these, heat conduction is the most serious loss mechanism... [1]."

Classic and neoclassical diffusion model the ion heat diffusivity using a random walk model of the ions and electrons as they move through their gyrokinetic trajectory around the magnetic field lines in the toroidal reactor, interacting with other charged species along their trajectory, and imparting thermal energy. Neoclassical transport theory refers to the diffusion process within a toroidal geometry, which generates for a 2.4 fold increase in ion heat diffusion.

The classical and neoclassical models are unable to account for the observed, anomalously large transport of energy and particles across the confining magnetic field. It is assumed that that the anomolous ionic thermal diffusivity is a function of various local dimensionless quantities, including β the ratio of plasma to magnetic pressure, ρ^*, which is explained below. Current research [2] focuses on plasma microturbulence caused by steep ionic thermal gradients as the driving mechanism for this anomalous heat transport, and incorporates scaling arguments in ρ^* to make predictions using available data from smaller scale fusion reactors to predict how ion heat diffusivity will scale to ITER levels. Scaling laws are laws used in fluid dynamics that are allowed to be made under dynamic and geomtric similarity situations, thus since the dynamics and geometries between tokamaks is nearly identical, scaling laws are useful when experimental validation is not available.

We define ρ^* to be $\rho^* = \rho_i/a$ where ρ_i is the gyrokinetic radius of the ion as it moves around the magnetic field in its trajectors through the fusion reactor, and a is the minor radius of the tokamak, or the radius of the inner cross-sectional area of the tokamak. The reason that ρ^* is interesting is because "Existing experimental devices can match all of these transport relevant dimensionless parameters expected in a reactor scale with the exception of ρ^* [4]." The inability to set the parameter rho^* in a lab experiment, and the advanced modeling and simulation capabilities of current tech, make a new study on ionic thermal diffusivity an ideal topic for a master's thesis

Thus, the stated purpose of this thesis is to determine how the ionic thermal diffusivity scales with a scan in ρ^* up to ITER scales, to determine whether the diffusion becomes Bohm or gyro-Bohm like. Bohm diffusion indicates that the diffusion increases linearly with temperature, and is undesireable, while gyro-Bohm diffusion indicates that the diffusion scales sublinearly with temperature, and is desireable.

We will use available experimental fusion reactor data, and implement surrogate modeling techniques to reduce the computational expense of running a simulation of 5-D gyrokinetic model of a plasma within a tokamak reactor, which is the geometr of the ITER reactor. The outcome of this project will be a pdf of the ion diffusion, with uncertainties. Once this is accomplished, if time permits, we will perform a comprehensive sensitivity analysis of the heating model.

1.3 Gyrokinetic Equations

The complete derivation of the governing set of equations of multi-scale physics in a tokamak reactor is well beyond the scope of this paper. However, the important physics that are described by the governing equations should be covered for clarity and reference. The governing set of equations of a plasma are called the Vlasov-Boltzmann equations and are provided below:

The first equation is the Boltzmann convection-collision equation modified for an electromagnetic system. Since the majority of the interactions in a plasma are Coulombic interactions, and they dominate the characteristics of the plasma, the collision term from the full Boltzmann eqution is ignored. The Vlasov equation decribes how the plasma is going to travel due to external forces acting on the plasma.

1.4 XGC Code & Heating Models

2 Experimental Metholodogy

3 Prediction under Uncertainty

Prediction under uncertainty is often an expensive and complicated process[5, 6]. 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[7, 8].

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.

3.1 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 $Q_S(\theta)$[9]. Sparse grid approaches [10, 11] 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[10].

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[8]. 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[10]. 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 [11]. 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 $Q(\theta)$.

3.2 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 [2]. 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.

3.3 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.

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4 Educational Methodology

In order to familiarize myself with the above experimental methods, I propose the following framework constructed of seeting up a toy problem, and implementing. 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 propogating the uncertainty of the parameters through the model to develop a distribtuion 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 [**?**].

After creating a blackbox to generate the quantity of interest under uncertainty, I can then use these generated quantities along with the avilable 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 of this information as a guiding example for the actual research being performed.

5 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.

Physics

A background in plasma physics, and the component of the XCG model that is used to model plasma heating and ion diffusivity. To support my physical understanding while completing this research I have identified the following references.

Plasma Physics and Fusion Reactors

[Jeffrey P. Friedberg Plasma Physics and Fusion Energy]

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.

Gyrokinetic Plasma Simulation

Plasma Modeling Methods and Applications - Textbook

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 good source for the developing and implementing the models that were discussed in the educational section of this proposal.

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 simualtion software. There is contact information available to constanct managing code users/developers.

Scaling Relationship Beween 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 clairty 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.

Gyroradius Scaling of Electron and Ion Transport - C.C. Petty et al

Prior Research in the Scaling Relationship Between χ_i and ρ^* Yasuhiro Idomura and Motoki Nakata has completed research in this field, analyzing the relationship between plasma size and ion temperature gradient driven turbulence. This scan was taken over sections comprised of 1/6 of the tokamak, with periodic boundary conditions.

Numerical Methodology

The mathematical component of my Master's of Integrated science will be fulfilled in this thesis 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

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 texbook has all of the background knowledge necessary to develop a toy surrogate model as proposed in this document.

Sparse Grids

Machine Learning

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.

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. Keih 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

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