# MIS Thesis Outline

### November 18, 2019

## 1 Introduction

Nuclear fusion confinement Nuclear fusion has the potential to be a clean, safe, cheap source of energy for the entire world. Nuclear fusion is the process that powers the sun, and is a highly energy favorable reaction. Thus, it makes sense that scientistis and engineers have been trying to understand and control nuclear fusion in a laboratory setting for the last 100 years.

Nuclear fusion is the process in which light elements, in our case of deuterium and tritium, have enough energy to overcome the Coulomb repulsion force, and get close enough together so that their nucleii fuse together. This results ini the formation of an  $\alpha$  particle, the release of a neutron, and the conversion of nuclear potential energy to kinetic energy. This release of kinetic is due to the decrease of potential energy in the nucleus as nucleons move closer to each other, thereby increasing the energy binding the nucleus together. The increase of kinetic energy during a fusion event is what motivates nuclear fusion research, as, at large enough scales, this process yields enough energy to be leveraged to power a steam turbine to produce electricity, potentially providing a clean, safe source of energy. Progress has been made in creating nuclear fusion reactors that can sustain a fusion plasma, one of the major issues of particular interest in this project is extending work that has been on understanding plasma size scaling of turbulent heat transport in future nuclear fusion devices. [1]



We are interested in nuclear fusion events that balance the likelihood of occurence and energy ouput after fusion. Considering these two factors, the reaction of primary interest in fusion research is the deuterium-tritium fusion reaction:

$$_{1}^{2}H + _{1}^{3}H \longrightarrow _{2}^{4}He + _{0}^{1}n,$$

where  ${}_{1}^{2}\mathrm{H}$  is deuterium (D), 3  ${}_{1}\mathrm{H}$  is tritium (T),  ${}_{2}^{4}\mathrm{He}$  is an  $\alpha$  particle, and  ${}_{0}^{1}\mathrm{n}$  is a neutron. Taking into account the binding energy of each element, the mass of the system before and after this nuclear fusion event is given by:

$$(2 - 0.000994) \,\mathrm{m}_p + (3 - 0.006284) \,\mathrm{m}_p \longrightarrow (4 - 0.0427404) \,\mathrm{m}_p + (1 + 0.001378) \,\mathrm{m}_p$$

where  $m_p = 1.6726*10^{-27} kg$  is the proton mass. The difference in mass before and after the reaction is thus  $\delta_m = -0.01875 m_p$ .

Using Einstein's famous equation  $\mathcal{E} = mc^2$ , where c is the speed of light, we find that energy-mass conversion to be

$$\mathcal{E} = \delta_m * c^2 = 0.01875 * 1.6726 * 10^{-27} kgc^2 = 17.9 MeV,$$

where the mass has been converted to kinetic energy. A further calculation shows that 1/5th of this energy is distributed to the  $\alpha$  particle, and the other 4/5th is distributed to the neutron. In a fusion reactor these two particles serve two important, and different, functions. When the number of fusion events is scaled to a large enough level, the resulting number of high energy neutrons can be leveraged to power a steam turbine, which through the inductive process, produces electricity. The high kinetic energy of the  $\alpha$  particles are used to increase the the kinetic energy of supplied D-T fuel, reducing the energy required for continuous external heating, creating a self-sustaining fusion process.

Since both deuterium and tritium have a net positive charge there is a repelling Coulomb force between them that prevents fusion from occuring in low temperature environments. Additionally in low temperature environments the cross sectional area of the D-T mixture is too low to make fusion an energy positive process. To overcome the Coulomb barrier, and increase the effective crosssection, the deuterium and tritium must be supplied enough kinetic energy to surpass the potential energy barrier to get within a particular radial distance from each other. "A positive energy balance is possible if the fuel particles can be made to interact to lose their energy. To achieve this the particles must retain their energy and remain in the reacting region for a sufficient time." This leads to a necessary confinement time of a sufficient number of particles within a particular region, or number density n, to create the conditions necessary for sustained fusion. The confinement time,  $\tau_E$ , is the primary parameter of interest in this project, as we are studying diffusive processes that degrade the experimental confinement time below the confinement time necessary for sustained fusion. In equillibrium, the kinetic energy of the D-T fuel mixture in a fusion reaction follows a Maxwellian distribution, and the high energy particles in the upper tail of the distribution are the source of the fusion reactions. The necessary average temperature to achieve desired fusion rates in this tail is 10keV, or around 100 million degrees centigrade. [1] The high temperature environment leads to complete ionization of the D-T mixture, yielding an equal number of electrons  $n_e$  and ions  $n_i$ . The net equality of charge leads to an electrically neutral system in equillibrium, which is highly responsive to external electric and magnetic fields; a gas in this state is referred to as a plasma. We would like to keep all of the fusion particles confined inside of the reactor, however the high energy and temperature of the plasma particles preclude using the physical wall of the reactor for confinement.[1] There are two important factors that must be considered when designing a device to confine a fusion plasma: the plasma state of the plasma the fact that we want to prevent the high energy particles of the plasma from colliding with the material walls of the device. Through the Lorentz force, the ions and electrons of the plasma can be confined with strong magnetic fields interior to the fusion device. A tokamak reactor is a toroidal nuclear fusion device that generates helical magnetic fields that provide a confining path for the ions and electrons of the plasma. The path traversed by the ions and electrons prior to reaching a material wall is a million times the length of the reactor.

#### Power Balance

For a fusion reactor to be viable from both an energy and economic persepective it must meet power balance condition:  $P_{out} >> P_{in}$ , where  $P_{out}$  is the power retrieved from the high energy neutrons, and  $P_{in}$  is the power necessary to sustain these fusion process while the reactor is in operation. [2] If the power necessary to sustain the fusion process is of the same order as the power recovered from the high energy neutrons, then our process will not be a worthy investment. Thus, understanding the input power  $P_{in}$  required to sustain nuclear fusion in a working scale tokamak reactor is of critical importance. Predicting  $P_{in}$  requires that we account for all of internal fusion plasma power sources,  $P_{source}$ , and powers sinks,  $P_{sink}$ , which we will do next. Once a full accounting of the sources and sinks is completed, the conditions necessary for a self-sustained fusion reaction can be determined.

The primary internal fusion power source are the  $\alpha$ -particles that are created during the fusion reaction. The magnetic fields generated by the fusion reactor confines the positively charged  $\alpha$ -particles. Under confinement, these  $\alpha$ -particles transmit the 3.5MeV they obtained during the fusion reaction to incoming D-T fuel, imparting enough kinetic energy for D-T fusion to occur. Taking into account  $\alpha$ -particle velocity, cross-sectional area as a function of velocity  $\sigma(v)$ , total ion density n, and energy per  $\alpha$ -particle,  $E_{\alpha}$ , the  $\alpha$ -particles heating or power per unit volume is

$$p_{\alpha} = \frac{1}{4}n^2 < \sigma v > E_{\alpha},$$

with  $\langle \sigma v \rangle$  being the fusion reaction rate assuming a Maxwellian distribution function. Integrating over the entire volume yields the total  $\alpha$ -particle power in the plasma.

$$P_{\alpha} = \int_{V} \frac{1}{4} n^{2} < \sigma v > E_{\alpha} d^{3} x$$
$$= \frac{1}{4} n^{2} < \sigma v > E_{\alpha} V.$$

with V being the volume of the reactor.

Now we account for power losses in the plasma. Due to temperature gradients and Coulomb collisions, in a tokamak reactor power is continuously leaving the plasma as ions and electrons move from the plasma to the reactor material walls. This lost power should ideally be completely replaced by  $\alpha$ -particle heating, and if it is not then external heating must be used to replace the lost power. "The average energy of plasma particles at a temperature T is  $\frac{3}{2}T...$ " [1]. The electrons and ions have the same temperaturee and quantitity, so if we let the ion number density per unit volume be n, the kinetic energy density of the system is 3nT. Integrating over the entire volume yields the following total plasma energy

$$W = \int_{V} 3nTd^{3}x$$
$$= 3\overline{nT}V.$$

We define the characteristic time  $\tau_E$  to be the amount of time that kinetic energy, once generated, stays in the plasma. This parameter is very important in nuclear fusion, as will be discussed below. Thus, the power lost is given by

$$P_H = \frac{W}{\tau_E}.$$

The total power balance equation is then given by

$$P_H + P_\alpha = P_L$$
 
$$P_H + \frac{1}{4} \overline{n^2 < \sigma v} > E_\alpha V,$$

where  $P_H$  is the applied heating power.

We now want to consider the power in a fusion reactor after fusion has been initiated. Is there a condition in the plasma that will yield enough  $\alpha$ -particle heating power to sustain the fusion process, and negate the need for external heating? Letting  $P_H = 0$  and rearranging the power balance equation yields the following inequality

$$n\tau_E > \frac{12}{<\sigma v>} \frac{T}{E_\alpha}.$$

Considering an operating temperature range of 10-20 keV,  $<\sigma v>=1.1\times 10^{-24}T^2m^3s^{-1}$ , yielding

the following condition for a self-sustaining plasma

$$nT\tau_E > 5 \times 10^{21} m^{-3} keVs$$

in which the density and temperature profile inside the plasma are parabolic, and n, T are the peak values of the profile. Given an operating temperature of 10 keV, and a number density of  $10^20m^{-3}$  yields a time constant of  $\tau_E = 5$  s, or the required energy confinement time in a tokamak reactor is around 5 s.

Confining energy in the plasma for the confinement time means that conditions must exist in the reactor that constrain heat from flowing at a rate faster than that dictated by the confinement time. In the 80s it was found that above sertain power levels the plasma transitions from a low energy mode (L-Mode) to a high energy mode (H-Mode), and in this high energy mode the confinement time of the plasma is reached. However, instabilities in the plasma edge, or edge localized modes (ELM) can cause the the plasma to crash from the H-mode back down to the L-mode. These edge localized modes are caused by turbulence driven transport, induced by ion temperature gradients in the plasma. flow must fully characterize all of the transport processes driving heat loss. A full characterization of the heat transport processes is beyond the scope of this master's report, but each of the transport mechanisms will be summarized here.

To motivate consider an exposed heat bath being used to maintain a solution in a beaker at a particular temperature in order to accelerate a chemical reaction (or personal bath that is being used to soak and relax in). (Possible diagrem here?). Our understanding of heat exchange tells us that the temperature difference, or thermal gradient, between the bath and the beaker will drive heat to travel from an area of high temperature to an area of low temperature, which in this case is the beaker soaking in the bath and the air directly above the bath. This transfer of hear raises the temperature of these heat sinks and lowers the temperature of the water. To maintain the temperature of the bath, the water will be kept in or on top of vessel that can act as a heat source, i.e. a hot plate, so that heat will continuously be added to the bath to compensate for heat loss.

Ideally the heat lost in this manner will not be so much as to require too much, or any external heating, especially. Calculating the rate at which heat leaves the system requires an understanding of how heat diffuses across the thermal gradient. In this example, heat transport is well understood - collisions between high energy/temperature water molecule and molecules in the beaker cause energy/momentum to be transferred from the water to the beaker and air. This energy transfer through collisions leads to an increase in temperature in the beaker, and eventually the solution it contains, the air above the heat bath, and reducing the temperature of the water.

( These calculations might be a bit too extreme for a personal bath, but would make sense in a lab where maintaining precise temperatures are necessary.

) This is an illustration of the principle of power balance - You have a system that has a required operating temperature. To maintain that temperature you must determine all of the ways that heat can be lost by accounting for all of the heat sinks, and the rates at which heat will be lost to the heat sinks through various heat transport mechanisms. This allows for the calculation of the rate at which heat must be added to system in order to counterbalance the heat being lost, and maintain the operating temperature of the system.

For a fusion plasma, balancing the heat loss is a tricky proposition. If enough heat is lost due to various heat transport mechanisms, using auxiliary heat The operating temperature of a fusion plasma is given by:t

Maintaining this operating temperature requires complete understanding of the rate at which heat is lost from the plasma. While the sinks are easily identifiable it turns out that, due to the fact that a plasma is a high temperature ionized gas subjected to an external magnetic field, understanding and describing the mechanisms that drive heat diffusion and convection to these sinks is quite complicated, and projecting the rate at which these mechanisms drive heat loss to the heat sinks at future reactors scales is still an unsolved problem. The work presented in this thesis is an attempt to contribute to the work already being done on this problem. Using advanced fusion plasma models, simulation code, and high-performance computing resources we are interested in

extending work that has been done to predict the rate at which heat is transported out of an ITER scale plasma through classical, neo-classical, and turbulence driven diffusion.

Due to the uncertainty in the heat deposition profile in the fusion plasma, as well as uncertainty due to discretization, and other paramaters in the heating model, we are interested in developing uncertainty bounds, or a probability distribution function, for the rate of rate diffusion out of plasma. This requires an understanding of which parameters are most strongly correlated with heat diffusion. Developing bounds on the uncertainty of in the heat diffusion parameter requires multiple runs of the above mentioned high-performance simulation code, which, due to computational expense, is currently an unfeasible proposition even with . Since computational resources are limited, we are interested in using existing data, or a limited number of full-fidelity simulations to develop a model surrogate for the full heating model, which will allow us to perform uncertainty quantification with an approximate model in a compurationally feasible manner.

In order to accurately predict power balance we must devise accurate models for where heat can be lost, or the power sinks, while a reactor is operating. in the reactor of In an ideal nuclear fusion reactor nothing is wasted: all of the kinetic energy of the high energy neutron is captured and either converted into electrical energy, or it is used in the tritium production process. Since alpha particles are charged, their momentum is transferred to incoming dueterium and tritium atoms via the Coulomb force, providing enough kinetic energy to cause them to fuse

and is primary fusion event of interest since it releases the most kinetic energy of all fusion events. Nuclear fusion of this type is more energetically favorable than all commonly used energy producing processes, including nuclear fission and combustion of hydrocarbons [1] (Friedberg). The energetic favorability of deuterium-tritium fusion has driven research in the field of nuclear fusion, with the goal of building a reactor that can start and sustain nuclear fusion in a manner that is overall energy positive. Additionally, there are less safety concerns about nuclear compared to nuclear fission reactors, since no enriched material has to be storedand the environmen(Environmental sustainability note here?) Predicting plasma size scalintransport in a fusion reactor is necessary for

We are interested in performing a simulation experiment that will provide uncertainty bounds on the rate at which energy, in the form of high energy ions, travels from the central region of tokamak fusion plasma towards the containing walls of the reactor. For the sake of staying consistent with the literature on fusion research we will refer to this flow of energy as heat or thermal transport, as the macroscopic temperature of a particular species of gas can be defined in terms of the of average kinetic energy of the species of gas, or:

$$E_{av} = \frac{n}{2}KT$$

Where  $E_{av}$  is the average kinetic energy of the gas species, n are the degrees of freedom of the gas species, K is Boltzmann's constant, and T is the temperature of the gas.

#### 1.1 Fusion Plasmas

The fusion event we interested in is Deuterium-Tritium fusion, during which the nucleus of a deuterium atom, D or  $^2\mathrm{H}$ , and the nucleus of a tritium atom,  $\mathrm{T}$  or  $^3\mathrm{H}$ , fuse together during the following nuclear reaction:

$$D + T \rightarrow {}^{4}\text{He} + n + 17.6 MeV.$$

The last term in this formula - 17.6 MeV- tells us that fusing the nucleus of a deuterium atom and a tritium atom converts 17.6 MeV of nuclear binding energy into kinetic-energy. In fact, the amount of energy generated per D-T fusion event rivals the energy per nuclear fission event, and just about every other energy producing process being leveraged at the moments.

Developing an entire theory of plasma transport is beyond the scope of this document. We will do
a brief review of plasma transport scaling from an experimental and simulation perspective. Discuss
the fact that, due to computational expense, no uncertainty quantification has been performed up
until this point on the simulations.

Here we discuss the baseline simulation, and the parameters that we are interested in propogating uncertainty through.

Here we will discuss surrogate models to overcome computational brute force expense of

## 2 XGC

Previous research in ion temperature gradient driven turbulence transport scaling has To perform the simulation of interest we use a full-f 5-D gyorxinetic simulation code. WE are able to reduce from 6-D to 5-D by averaging over the the saft time scale of the gyrkinetic motion  $\delta f$  simulations. Full-f simulations evolve the entire ion and electron distribution function, rather than fixing a background distribution and evolving a perturbed distribution according to the physical model, or a  $\delta f$  simulation. The reason we use such an approach is that in the edge region of the plasma that we are interested in simulating the perturbation amplitude reaches  $\delta f/f_0\mathcal{O}(1)$ 

leading to a p

Confinement Tokamaks

To motivate the driving question being investigated in this thesis, consider an exposed heat bath being used to maintain a solution in a beaker at a particular temperature in order to accelerate a chemical reaction (or personal bath that is being used to soak and relax in). (Possible diagrem here?). Our understanding of heat exchange tells us that the temperature difference, or thermal gradient, between the bath and the beaker will drive heat to travel from an area of high temperature to an area of low temperature, which in this case is the beaker soaking in the bath and the air directly above the bath. This transfer of hear raises the temperature of these heat sinks and lowers the temperature of the water. To maintain the temperature of the bath, the water will be kept in or on top of vessel that can act as a heat source, i.e. a hot plate, so that heat will continuously be added to the bath to compensate for heat loss. Ideally the flow of hot water in would perfectly match the flow of heat out of the bath, so that the temperature of the bath stays constant. Calculating

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an approximate model in a computationally feasible manner.

### 2.1 Magnetically Confined Fusion

#### 2.1.1 Nuclear Fusion Introduction

Importance of fusion as an energy source.

Physical description of nuclear fusion and how it relates to a plasma.

## 2.1.2 Important Plasma Definitions

Debye Shielding

Plasma Frequency

Group Behavior

#### 2.1.3 Development of physics relevant to simulation and work

General Behavior of Charged Particles in an Electric and Magnetic Fields. Drift phe-

nomenon. Magnetic Confinement Principles. Traveling waves in a plasma. Kinetic Theory Heating

Model. Heat transport - Classical, Neoclassical, and Turbulent Transport.  $\rho*$  scaling.

Methodology used to understand and predict heat transport at ITER scales: Experimentation and simulation to develop scaling laws of dimensionally similar systems.

## 2.2 Plasma Simulation Description - XGC Code

Importance of simulations, what they allow us to understand and predict on.

Computational expense of modern plasma simulations.

## 2.3 UQ as a way to build a PDF on QOI from a plasma simulation

Full description of sources of uncertainty in simulation - I.E. uncertainty of input parameters, variables

Description of propagation of error through a forward non-linear map. Give basic example here using the nonlinear Landau damping UQ example.

## 2.4 Surrogate Modeling

What is a surrogate model? How can surrogate models be helpful when performing Hi-Fi plasma simulations. Examples. How do we develop a surrogate model? Be very clear here.

# 3 Literature Review

Complete this weekend - stop hemming and hawing as Mike would say Summarize Idomura Paper

- 3.1 Landau Damping Derivation and Physical Meaning?
- 3.2 Neoclassical Theory, Scaling Laws, and Diffusion Still Relevant? A lot of reading and work was done on this. Perhaps substitute for Landau Damping, or use Landau Damping as a test case for UQ to illustrate what we intend to do.
- 3.3 Gyrokinetic Equations Still relevant?
- 3.4 XGC code & Heating Model
- Still relevant? Code is installed on Theodon.
- 3.5 Surrogate models in UQ
- 4 UQ test case Landau damping both linear and non-linear regimes. Experimental methodology
- 5 3

Simulation-"Experimental Methodology"

- 6 Results
- 6.1  $\rho$ \* Scaling
- 6.2 Sensitivity to deposition profile
- 7 Conclusions