GA–A27704

STEADY-STATE GYROKINETICS TRANSPORT CODE (SSGKT)

A Scientific Application Partnership with the Framework Application for Core-Edge Transport Simulations

Final Report

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DISCLAIMER

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Work supported by
the U.S. Department of Energy
under DE-FC02-07ER54921

GENERAL ATOMICS PROJECT 30015
NOVEMBER 2013

GENERAL ATOMICS

Abstract

This project initiated the development of TGYRO — a steady-state Gyrokinetic transport code (SSGKT) that integrates micro-scale GYRO turbulence simulations into a framework for practical multi-scale simulation of conventional tokamaks as well as future reactors. Using a lightweight master transport code, multiple independent (each massively parallel) gyrokinetic simulations are coordinated. The capability to evolve profiles using the TGLF model was also added to TGYRO and represents a more typical use-case for TGYRO.

Background

The goal of the project was to develop a steady-state Gyrokinetic transport code (SSGKT) that integrates micro-scale gyrokinetic turbulence simulations into a framework for practical multi-scale simulation of a burning plasma core - the International Thermonuclear Experimental Reactor (ITER) in particular. This multi-scale simulation capability will be used to predict the performance (the fusion energy gain, Q) given the H-mode pedestal temperature and density. At present, projections of this type rely on transport models like GLF23, which are based on rather approximate fits to the results of linear and nonlinear simulations. Our goal is to make these performance projections with precise nonlinear gyrokinetic simulations. The method of approach is to use a lightweight master transport code to coordinate multiple independent (each massively parallel) gyrokinetic simulations using the GYRO code.

This project targets the practical multi-scale simulation of a reactor core plasma in order to predict the core temperature and density profiles given the H-mode pedestal temperature and density. A master transport code will provide feedback to O(16) independent gyrokinetic simulations (each massively parallel). A successful feedback scheme offers a novel approach to predictive modeling of an important national and international problem. Success in this area of fusion simulations will allow US scientists to direct the research path of ITER over the next two decades.

The design of an efficient feedback algorithm is a serious numerical challenge. Although the power source and transport balance coding in the master are standard, it is nontrivial to design a feedback loop that can cope with outputs that are both intermittent and extremely expensive. A prototypical feedback scheme has already been successfully demonstrated for a single global GYRO simulation, although the robustness and efficiency are likely far from optimal. Once the transport feedback scheme is perfected, it could, in principle, be embedded into any of the more elaborate transport codes (ONETWO, TRANSP, and CORSICA), or adopted by other FSP-related multi-scale projects.

Deliverables

GYRO and TGYRO are released and available online (at General Atomics web site). An overview of the TGYRO project is given at

http://fusion.gat.com/theory/Tgyrooverview with user documentation given at

http://fusion.gat.com/theory/Tgyrousermanual

Regarding the integration of SSGKT with FACETS, an advanced interface to the GYRO code was developed and released. This interface allowed the GYRO code to be called from the FACETS code directly, which allows for *time-dependent* steady-state transport simulations using a first-principles turbulence code with fluxes. The ability to do time-dependent studies is a feature not present in the prototype TGYRO. The interface is documented at

http://fusion.gat.com/theory/Gyroinput

However, continual development of physics needs within the FACETS project may lead to the FACETS team doing further modifications to the GYRO/FMCFM interface.

The original science goals have been met: By incorporating improvements to the TGYRO iteration scheme, we have been able to compute steady-state temperature profiles for DIII-D L-mode discharge 128913. Computational and experimental results compare remarkably well over the simulation domain, with the dominant discrepancy occurring in the electron temperature near the magnetic axis. This result represents perhaps the most comprehensive kinetic code validation exercise ever attempted, and complements the traditional validation approach, which focuses on flux rather than profile comparison. The present quality of agreement gives us confidence that the TGYRO approach will be the most accurate available for ITER performance predictions.

Approach

Presently, at the macro-scale end of the spectrum, predictive modeling of steady-state temperature and density profiles [8] is usually done with local transport models like GLF23. These transport models are based on approximate fits to external simulation datasets. Conversely, at the micro-scale end the spectrum, the ubiquitous approach in the gyrokinetic simulation community is to compute the statistical steady-state of turbulence which is generated by fixed plasma profiles. Indeed, GYRO is regularly used for relatively inexpensive fixed-profile simulations (i.e., without feedback) of global DIII-D, JET, C-Mod and NSTX experiments. Such simulations are far shorter than the global transport (energy confinement) time. By separating the turbulence (internal, micro-scale physics) and transport (external, macro-scale physics) time scales, and introducing a feedback loop between them, one can arrive at the steady-state transport balance required for a true macro-scale steady-state solution.

The TGYRO method of approach, in short, is to use a lightweight master code to coordinate feedback between a transport module and multiple separate GYRO gyrokinetic simulations. This approach will allow highly efficient use of very large processor counts (several thousand); the master code must only compute relatively simple feedback information based on transport power balance, and the independent instances of GYRO will scale very well because of the relatively low processor count per instance (32 to 256). Each instance of GYRO will compute local radial fluxes that will be periodically communicated to the master. In comparison to the size of a local simulation distribution function, the amount of data to be communicated to the master will be minimal. The transport module, and in particular the feedback scheme (or schemes) it will employ, have not yet been developed. However, the physical sources (beam ions, radio frequency (RF) heating, radiation, thermonuclear rates, etc.) which must be accounted for in the master are available as off-the-shelf technology. The use of the transport power and plasma flow balance equation, rather than direct dynamical interactions, is potentially the key solution to connecting core turbulence to the edge pedestal.

Progress over the Three Year Project

2009

The interface code to be able to call GYRO from FMCFM, and thus FACETS, was completed. A key component to any interface is a complete understanding of how to convert the variables from one component to the other. A conversion mapping was established and documented. We found that some basic geometry variables needed to be added to FMCFM, and as a by-product we have helped improve the FMCFM framework. The conversion mapping and the interface code are complete.

It has been understood that machine precision differences with respect to initial conditions of a GYRO simulation can lead to order unity differences in instantaneous diffusivities. This requires the user to use a time history average of the simulation period (beyond a suitable initial transient phase) to obtain statistically calculated diffusivities. Using this averaging allows one to state that the results from our benchmark tests agree, thus demonstrating that the FMCFM package correctly builds a GYRO library that is correctly interfaced to the standalone GYRO driver BigScience.

The second step of the benchmarking task was to ensure that all conversions from FMCFM units to GYRO units are consistent, including all input parameters for GYRO. This was successfully demonstrated as well. A fortran driver using the native data structures of FMCFM is able to reproduce results from the standalone GYRO built within the FMCFM build system.

The final stage of embedding GYRO within the FACETS framework tested GYRO when called via FMCFM from the FACETS framework. Extensive work by A. Hakim in creation of C++ transport classes has allowed for encapsulation of FMCFM c-callable “setters and getters” via a Fortran opaque handles.

Steady-state algorithm development accomplishments (General Atomics)

Significant development and improvement of the core physics capability of TGYRO has occurred, by General Atomics. TGYRO can control execution of the gyrokinetic code GYRO, the TGLF transport model, the QFM (Weiland) transport model, as well as the kinetic neoclassical code NEO. When maximum realism is required, GYRO can be used to compute the turbulent flux, and NEO to compute the neoclassical flux.

Locally, test runs showed that with this combination, TGYRO can scale successfully up to 122,880 cores! Also, physics upgrades to the GYRO code, including a more accurate collision operator, more accurate rotation and rotation shear physics, as well as the capability for high-accuracy up-down asymmetric equilbria, can now be utilized by TGYRO.

By incorporating improvements to the TGYRO iteration scheme, we have been able to obtain steady-state temperature profiles for DIII-D L-mode discharge 128913. Computational and experimental results compare remarkably well over the simulation domain, with the dominant discrepancy occurring in the electron temperature near the magnetic axis. This result represents perhaps the most comprehensive kinetic code validation exercise ever attempted, and complements the traditional validation approach, which focuses on flux rather than profile comparison. The present quality of agreement gives us confidence that the TGYRO approach will be the most accurate available for ITER performance predictions.

The results for DIII-D shot 128913 were published in Physics of Plasmas (June 2009), and also presented at the 51st APS meeting in Atlanta, GA.

2008

Much time was spent on getting GYRO into the FACETS framework this year. More specifically, GYRO will be incorporated into the Framework for Modernization and Componentization of Fusion Modules (FMCFM), which facilitates access to transport modules from integrated modeling codes.

The first stage was to make the GYRO build system work under “autotools” and at the same time within the FACETS build system, which has been completed. Now, configuring and building FACETS also builds GYRO. Considering GYRO did not use “autotools” previously to build and the PI for this work never wrote “autotools” code before, this effort took several months to complete.

The second stage of this work was to write interface code to be able to call GYRO from FMCFM, and thus FACETS. A key component to any interface is a complete understanding of how to convert the variables from one component to the other. A conversion mapping is underway, and we are finding some basic geometry variables need to be added to FMCFM, and as a by-product we are helping to improve the FMCFM framework. Although the conversion mapping is not yet complete, we have started writing some interface code. We are hopeful of completing the interface code in November.

2007

One of the first milestones was to research code-coupling strategies and implement an initial choice. This was completed within the first 3-6 months of the project. Although there are several code-coupling strategies and frameworks, we chose for simplicity to stay within the "Fortran90" programming environment and use Fortran90 modules to "exchange" data. The first task was to modify the existing production code GYRO so as to encapsulate its data within gyro-only F90 modules. Then a "master" code was written in Fortran90 that will be used to coordinate multiple GYRO instances and with a transport module. Thus, a prototype is in place, although we may revisit the code-coupling implementation at a later date.

The prototype code, TGYRO, has been implemented and tested on several platforms. This prototype couples multiple instances of GYRO together (which will give us the ability to scale to many thousands of processors) and implements a feedback loop between turbulence and transport - the transport part of the prototype is an overly simplified model, but will become more realistic in the next year as originally planned. TGYRO currently supports two "modes" of feedback operation: (a) local and (b) global. The local method employs a different flux-tube simulation at every radius, while the global method uses feedback at all radii on a single global simulation. The local method is suitable for reactor-scale plasmas, whereas the global method is suitable for existing experiments.

Local Mode
We have done preliminary testing with the TGYRO prototype in local mode, with results yielding smooth profiles and an overall proof-of-principle of the method. For example, with 4 instances of GYRO at the radii r=(0.2, 0.4, 0.6, 0.8) and 16 processors per instance, we get the steady-state profiles seen in Figure 1 (will be included in later document). A GA post-doc was recently hired and is just now adding "toy model" (the so-called IFS-PPPL model) capability for the transport fluxes to TGYRO as a development tool. This will enable benchmarking of the basic iteration scheme and results with the GLF/XPTOR transport code at GA. Note that there was a significant delay in hiring the postdoc because GA did not receive project funds until approximately April 2007.

Global Mode
Basic capability for global feedback operation has been added and we are in the process of moving the global feedback algorithm (developed by R. Waltz) from a development version of the GYRO code to the TGYRO framework.

We have presented a few talks and included our status in a SciDAC article on the FACETS project.

Publications

2009 Publications
J. Candy, C. Holland, R. Waltz, M. Fahey and E. Belli, “Tokamak profile prediction using direct gyrokinetic and neoclassical simulation,” Phys. Plasmas **16**, 060704 (2009)

J R Cary, J Candy, J Cobb, R H Cohen, T Epperly, D J Estep, S Krasheninnikov, A D Malony, D C McCune, L McInnes, A Pankin, S Balay, J A Carlsson, M R Fahey, R J Groebner, A H Hakim, S E Kruger, M Miah, A Pletzer, S Shasharina, S Vadlamani, D Wade-Stein, T D Rognlien, A Morris, S Shende, G W Hammett, K Indireshkumar, A Yu Pigarov and H Zhang, "Concurrent, parallel, multiphysics coupling in the FACETS project," SciDAC 2009, J. Physics: Conf. Series 180, 012056 (2009).

J. Candy, C. Holland, R. Waltz, M. Fahey and E. Belli, “Tokamak profile prediction using direct gyrokinetic and neoclassical simulation,” General Atomics Report GA-A26380, February 2009 (submitted to PRL).

2009 Presentations
J. Candy, “Predictive Gyrokinetic Transport Simulations and Application of Synthetic Diagnostics”, invited oral presented at the 51st APS-DPP meeting, Atlanta, GA, 2-6 November 2009.

J. Candy, “Status of GYRO/NEO/TGYRO,” lecture presented at Scientific Grand Challenges in Fusion Energy Sciences and the Role of Computing at the Extreme Scale, Washington, D.C., 18-20 March 2009.

2008 Publications
J. Candy, H. Nordman, M. Fahey, T. Fulop and E. Belli, “Transport in ITER-like plasmas in neoclassical, fluid and gyrokinetic descriptions,” paper TH/P8-28, submitted to the 22nd IAEA Fusion Energy Conference, Geneva (Oct 2008).

2008 Presentations
J. Candy, M.R. Fahey, R.E. Waltz and T. Fouquet, “Progress on TGYRO: The Steady-state Gyrokinetic Transport Code,” poster presented at the 21st US Transport Taskforce Workshop, 25-28 March 2008.

T. Fouquet, J. Candy, M.R. Fahey and R.E. Waltz, "Progress on TGYRO: the steady-state gyrokinetic transport code," poster presented at the 2008 International Sherwood Fusion Theory Conference, Boulder, CO, 30 March - April 2 2008.
J. Candy, R.E. Waltz, M.R. Fahey, E. Belli, "Gyrokinetic and Neoclassical Transport Modeling for ITER: Selected Results," presented at UCLA, Los Angeles, CA, 3 April 2008.
J. Candy, R.E. Waltz, M.R. Fahey, E. Belli, "Gyrokinetic and Neoclassical Transport Modeling for ITER: Selected Results," presented at Chalmers University, Sweden, 26 May 2008.

2007 Presentations
"Status on the computational aspects of developing a fully gyrokinetic transport code," M.R. Fahey, J. Candy, and R. Waltz, presented at the Transport TaskForce Workshop, San Diego, April 2007, http://fusion.gat.com/conferences/ttf/files/poster/core/Fahey_poster.pdf

"Progress on a Fully Gyrokinetic Transport Code," J. Candy, M.R. Fahey, and R. Waltz, presented at Transport TaskForce Workshop, San Diego, April 2007

"Progress on a Fully Gyrokinetic Transport Code," J. Candy, M.R. Fahey, and R. Waltz, presented at 2007 European Physical Society Meeting, Warsaw, Poland, July 2007

"Introducing FACETS, the Framework Application for Core-Edge Transport Simulations," J.Cary, et al., proceedings of SciDAC 2007, Boston, MA, June 2007.