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Small Business Name: CompX

Business Official (BO) Name: R.W. Harvey

BO Email Address: rwharvey@compxco.com

BO Phone Number: 858-509-2131

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Four-Dimensional Finite-Orbit-Width Fokker-Planck Code with Sources, for Neoclassical/Anomalous Transport Simulation of Ion and Electron Distributions

Principal Investigator (PI) Name: R.W. Harvey, rwharvey@compxco.com

Team Members: Drs. R.W. Harvey, Yu.V. Petrov (CompX), with subcontractors.

Subcontractors: Drs. X. Xu & M. Dorf, Lawrence Livermore National Laboratory

Limitations on Distribution: None

Executive Summary of

Four-Dimensional Finite-Orbit-Width Fokker-Planck Code with Sources, for Neoclassical/Anomalous Transport Simulation of Ion and Electron Distributions, SBIR Phase I Award DE-SC0009491

Within the US Department of Energy/Office of Fusion Energy magnetic fusion research program, there is an important whole-plasma-modeling need for a radio-frequency/neutral-beam-injection (RF/NBI) transport-oriented finite-difference Fokker-Planck (FP) code with combined capabilities for 4D (2R2V) geometry near the fusion plasma periphery, and computationally less demanding 3D (1R2V) bounce-averaged capabilities for plasma in the core of fusion devices. Demonstration of proof-of-principle achievement of this goal has been carried out in research carried out under Phase I of the SBIR award. Two DOE-sponsored codes, the CQL3D bounce-average Fokker-Planck code in which CompX has specialized, and the COGENT 4D, plasma edge-oriented Fokker-Planck code which has been constructed by Lawrence Livermore National Laboratory and Lawrence Berkeley Laboratory scientists, where coupled. Coupling was achieved by using CQL3D calculated velocity distributions including an energetic tail resulting from NBI, as boundary conditions for the COGENT code over the two-dimensional velocity space on a spatial interface (flux) surface at a given radius near the plasma periphery. The finite-orbit-width fast ions from the CQL3D distributions penetrated into the peripheral plasma modeled by the COGENT code. This combined code demonstrates the feasibility of the proposed 3D/4D code.

By combining these codes, the greatest computational efficiency is achieved subject to present modeling needs in toroidally symmetric magnetic fusion devices. The more efficient 3D code can be used in its regions of applicability, coupled to the more computationally demanding 4D code in higher collisionality edge plasma regions where that extended capability is necessary for accurate representation of the plasma. More efficient code leads to greater use and utility of the model. An ancillary aim of the project is to make the combined 3D/4D code user friendly.

Achievement of full-coupling of these two Fokker-Planck codes will advance computational modeling of plasma devices important to the USDOE magnetic fusion energy program, in particular the DIII-D tokamak at General Atomics, San Diego, the NSTX spherical tokamak at Princeton, New Jersey, and the MST reversed-field-pinch Madison, Wisconsin. The validation studies of the code against the experiments will improve understanding of physics important for magnetic fusion, and will increase our design capabilities for achieving the goals of the International Tokamak Experimental Reactor (ITER) project in which the US is a participant and which seeks to demonstrate at least a factor of five in fusion power production divided by input power.

Comparison of Actual Achievements in Phase I with Project Goals

The original objective of Phase I was to upgrade certain features of the TEMPEST 4D (2R-2V) finite difference gyro-kinetic code [Xu, 2007], a precursor code to the 4D COGENT [Dorr, 2010] code. TEMPEST was more fully developed as a physics and computational model, but had drawbacks which led to a new project for the COGENT code. CompX first targeted TEMPEST as a companion 4D Fokker-Planck model to its well-established CQL3D code, with the stated intention to use methods developed with TEMPEST for future work with COGENT. However, TEMPEST had not been used for about four years. After substantial work on recommissioning TEMPEST with currently available supporting libraries, it was determined that this was not possible within the bounds of the Phase I SBIR. Therefore, CompX refocused its effort on the COGENT code. By doing this, a substantial portion of the original Phase I proposal objectives could be met. In particular, Phase I objectives were [Phase I, but with TEMPEST replaced by COGENT]:

1. Develop/verify operation of COGENT as a full-radius transport code.
2. Update/modify collisional operator in COGENT based on latest fully-nonlinear relativistic collisional operator from CQL3D.
3. Add Ampere-Faraday equations for self-consistent toroidal electric field.
4. Improve/accelerate job runs of TEMPEST with preconditioning of the main equation set matrix.

We were able to (1) verify COGENT running as essentially a full-radius code, by extending to operate over 99.8% of the plasma cross-section, omitting the small volume near the plasma magnetic axis (which can be addressed in Phase II); (2) The COGENT collision operator has been upgraded to a fully nonlinear collision operator of the type in CQL3D (except non-relativistic) [Dorf, 2013]; (3) An Ampere-Faraday equation implementation is being tested in CQL3D [Harvey, 2013] and similar methods may be applied to COGENT; (4) The COGENT team is examining code speed up through implementing time-implicit equation advancement.

Additionally we have achieved a direct coupling of COGENT and CQL3D as will be shown below. This latter result validates the possibility of full-radius gyrokinetic Fokker-Planck plasma modeling using the more computationally intense 4D COGENT code in high collisionality plasma periphery as required by the physics, coupled to the faster CQL3D code in the low-collisionality core code, where bounce-averaging is suitable.

Importantly, the Phase I work has enabled development of a strong collaboration of the CompX team with COGENT developers at Lawrence Livermore National Laboratory and at Lawrence Berkeley Laboratory.

Technical Description of Accomplishments During SBIR Phase I

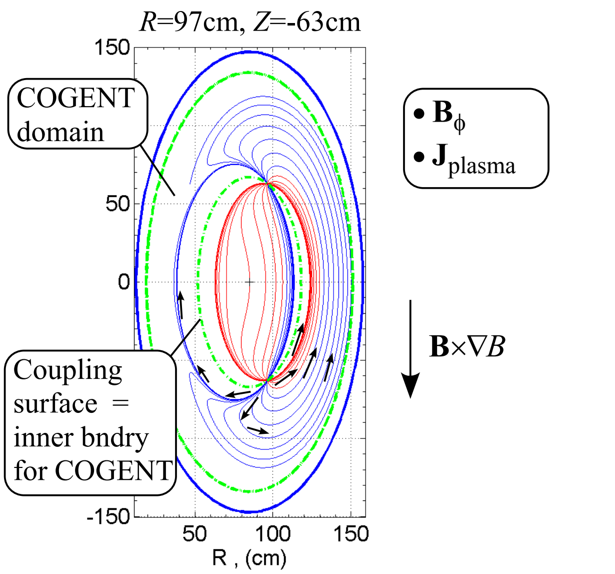

Fig. 1. Orbits of 30 keV D^+ ions coming from the coupling boundary r/a=0.5 into the COGENT domain (between the two dashed lines). Blue orbits: particles injected with $V_{||}<0$, red: with $V_{||}>0$. The bold blue ellipse designates the vacuum chamber.

The main goal of Phase I was to demonstrate the feasibility of coupling between the CQL3D and a 4D gyro-kinetic code. The initial efforts were focused on the 4D TEMPEST code [Xu, 2007]. It was found, however, that because of lack of maintenance in past several years, and because the code infrastructure is based on presently obsolete external libraries, the code cannot be run on NERSC supercomputers in it's original shape. It was realized that bringing the code into a working condition would require much more time than it was available in Phase I; as a result, we switched our focus to another 4D/5D gyro-kinetic code – COGENT, which was mentioned in Phase I proposal as an alternative. The COGENT code is in active stage of development at LLNL, and we were able to obtain a helpful assistance for installation, modifications and running the code.

In Phase I period of this work, CompX, along with the help of Drs. M. Dorf and R.H. Cohen (retired) from LLNL, have shown proof-of-principle coupling of CQL3D and COGENT in a relatively simple toroidal geometry, based on analytical Miller equilibrium [Miller, 1998]. As a test, the distribution function for the central area of plasma (r/a < 0.5) was found by the CQL3D code, with NBI sources originating from r/a < 0.5 area only. As an example, we analyzed a calculated distribution function at the midplane within the COGENT domain. From Fig. 1 of 30 keV D^+ orbits it is seen that the ions flowing from the coupling surface into the 0.5<r/a<1 of COGENT domain can only contribute to the co-current part of the local distribution function at the outer-board/midplane. The initially co-current particles that start at (R=97cm, Z= –63cm) remain co-current at the midplane (red color). The counter-current passing particles (several blue elliptical orbits)

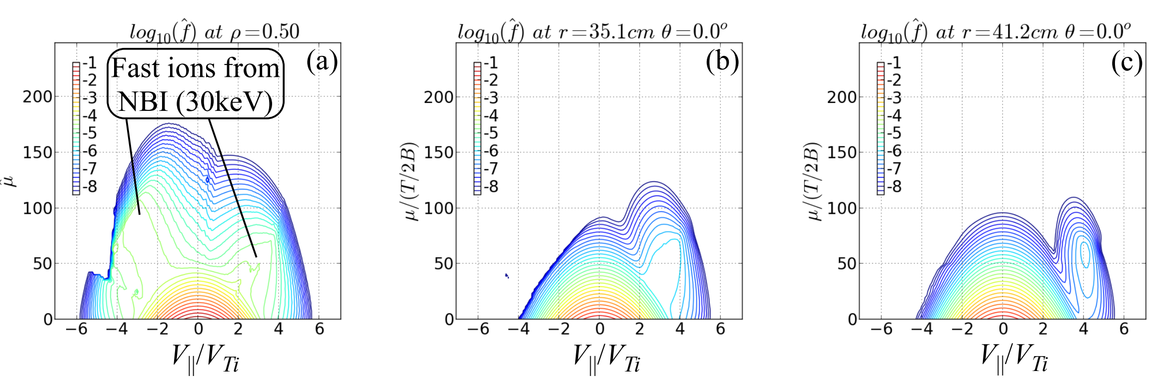

Fig. 2. (a) Local distribution function from CQL3D, in normalized ($V_{||}$,μ) coordinates, set at r=33cm (r/a=0.5) coupling radius; (b,c) Distribution function obtained by COGENT at t=6×10^{-6} sec (≈τ_{bounce} for fast ions), shown for two selected radial points at the outerboard/midplane region. The initial distribution at r/a>0.5 is set to be Maxwellian with T = 1 keV, n_e= 3×10^{19} m^{-3}.

can only travel to the inner-board region. The trapped particles that start with $V_{\|}<0$ (blue curves) bounce at smaller R and then cross the midplane with $V_{\|}>0$, therefore also contributing to the co-current part of the distribution at the midplane. This picture was confirmed by the shape of solution obtained with COGENT, as seen in Fig.2(b,c).

The flow of particles shown in Fig. 1 also leads to ideas of how the two codes can be coupled. It is clear that the lower part of the coupling surface (for a given direction of **B**) serves as an "emitting" border, while the upper part serves as an "absorbing" border, as viewed by the COGENT domain. In the absence of collisions or other interactions of particles in the COGENT domain (such as scattering by turbulence), the distribution function at the upper border should be exactly the same as in the lower "emitting" border. This is demonstrated in Fig. 3, where the boundary condition at the coupling surface is set in the CQL3D distribution as a localized source with non-zero distribution present at narrow range in poloidal angles (≈280º), energies (≈30 keV), and pitch-angles (≈0.55π). The initial distribution in COGENT domain is set to zero. Such boundary condition represents an orbit (or rather, a set of similar orbits) that starts with $V_{\|}<0$, but quickly bounces and travels upward with $V_{\|}>0$. The solution found by COGENT becomes up/down symmetric and steady-state after ≈1500 time steps. It should be noted that both the boundary distribution and the interior distribution are affected by the grid sizes. In calculations for Fig.3, the size of radial grid is 16 nodes, and poloidal grid – 64 nodes. If the size of poloidal grid is reduced in half, the density "packet" widens during propagation through the COGENT domain, resulting in about 5% wider poloidal angle localization at the upper border point than at the lower ("emitting") point.

In case when a collisional or other diffusive processes are added to the 4D Fokker-Planck equation in the COGENT domain, the up/down symmetry is broken. From the CQL3D point of view, an orbit with given COM, corresponding to the "emitted" distribution, is annihilated within COGENT domain, but at the same time another orbit (or a set of orbits) with a different COM is produced within COGENT domain. The effect of COGENT-based modifications can be accounted by comparing the

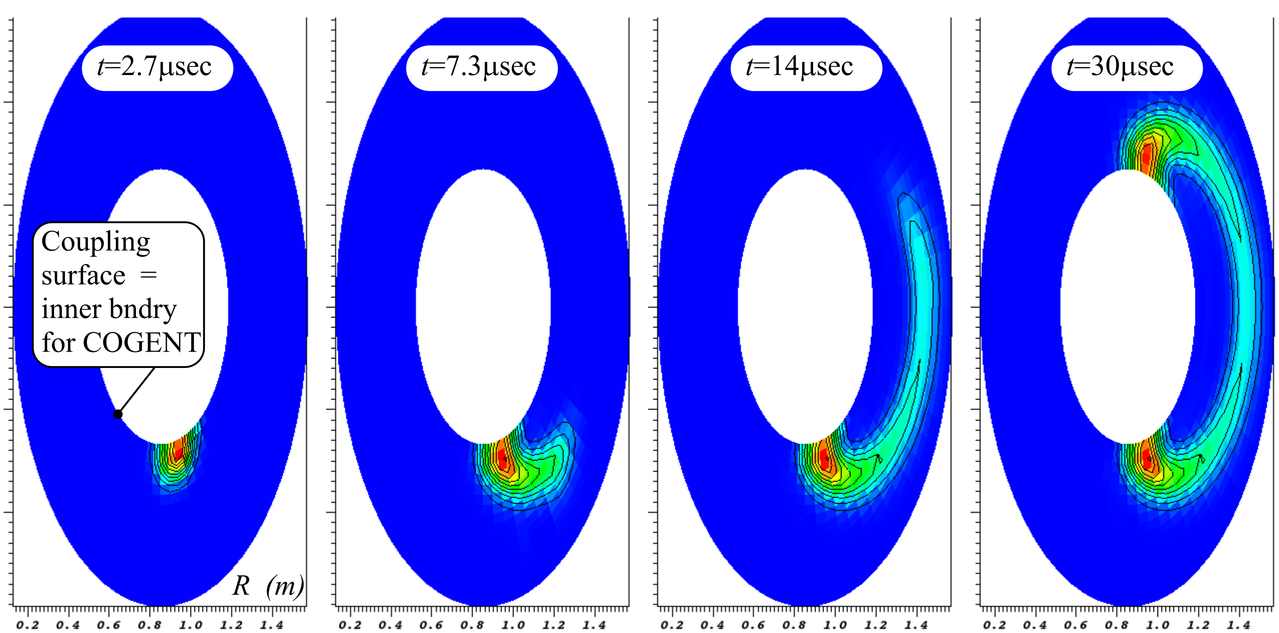

Fig. 3. Change of particle density calculated by COGENT. Initial distribution in COGENT domain is zero (blue area). The inner-boundary condition is a delta-type distribution function localized in poloidal angle, energy and pitch-angle. The solution found by COGENT becomes up/down symmetrical and steady-state after t≈25μsec (1500 time steps).

distribution function at the upper border (f_{COGENT}) with the original boundary distribution obtained from CQL3D (f_{CQL3D}). The bounce-average FPE in the CQL3D code should be adjusted by introducing the source/sink term in shape of

$$(\partial f/\partial t)_{source/sink} = (f_{COGENT} - f_{CQL3D})/\tau_{bounce}.$$

For example, if all orbits emitted from the lower border are lost to the chamber wall while traveling in the COGENT domain, then at the upper border $f_{COGENT}=0$, so that

$$(\partial f/\partial t)_{source/sink} = -f_{CQL3D}/\tau_{bounce} ,$$

which is a sink term that pushes the distribution to zero in one bounce time.

The source/sink term should be evaluated for each node of the 3D grid in CQL3D computational space, by mapping f_{COGENT} and f_{CQL3D} from the coupling boundary back to the midplane where the CQL3D computational grids are defined. By incorporating the $(\partial f/\partial t)_{source/sink}$ term, a new solution is obtained in the CQL3D domain, thus yielding the updated boundary condition for COGENT. It should be noted that the computational time needed for updating the CQL3D solution is negligible comparing to that required by COGENT, so the strategy in coupling the codes would be reducing the COGENT domain to an edge region as small as possible.

Among other tasks performed during Phase I was testing/verification of the COGENT as a nearly full-radius transport code. For conditions used in the above figures, the inner coupling radius could be reduced to r_c=3cm, which contains only ≈0.2% of the plasma volume. The limitation comes from the singularity in metric coefficients related to mapping from the (r, θ_{pol}) physical grid to the computational rectangular grid. In the view of our coupling strategy, this limitation does not appear to be an issue.

The modification of the collision operator, which was a planned task for the TEMPEST code, was not needed for COGENT. It has several options for collisions that are well tested [Dorf, 2013a]. The recent addition is the fully-nonlinear collision operator [Dorf, 2013b]. In initial tests, a relaxation to a Maxwellian distribution is demonstrated, with second-order accuracy in energy conservation. The main concern with the collision (and other diffusive processes) operator is a constrain on the time step, which can become much smaller than that dictated by a simple transit-time over a grid-cell condition. To address this issue, a possibility of an implicit integration is being considered, which would allow to set the time step even larger than the transit time.

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