DOE Final Report on Virginia Tech's contribution to "Tokamak Disruption Simulation"

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On behalf of work completed while Author was PI at Virginia Tech

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Grant number: DE-SC0018276

Performance period: 09/01/2017 to 08/31/2024 (with a no-cost extension)

1 Introduction and overview

This work was performed by Virginia Tech in collaboration with multiple institutions led by Los Alamos National Laboratory as a part of the Tokamak Disruption Simulation SciDAC (Scientific Discovery through Advanced Computing) project supported jointly by the Department of Energy Office of Science and Advanced Scientific Computing Research. This report summarizes Virginia Tech's contributions to the SciDAC project. Virginia Tech researchers (presently University of Washington researchers) focused on the fundamental role of plasma-material interaction on transport, which could then have macroscopic effects on simulations of tokamak disruptions. The plasma sheath, which regulates plasma particle and energy fluxes to the wall, is an essential component in the study of plasma-material interaction (PMI). Understanding sheath theory by accounting for finite sheath thickness and transport in the vicinity of the sheath entrance can significantly modify typical assumptions that are made in the Bohm speed analysis, where the Bohm speed provides the lower bound of the plasma exit flow speed. Our work provides a modified Bohm speed formulation that accounts for the critical role of transport and for applications that are away from the asymptotic limits that are typically assumed.

The Los Alamos National Laboratory code, VPIC, was developed further to incorporate the necessary collisional physics into the eletromagnetic particle-in-cell model. VPIC is a highly efficient particle-in-cell code that has been extensively benchmarked for a number of kinetic applications and has been applied to a number of sheath studies as well. Simultaneously, a continuum-kinetic approach was pursued using the Princeton Plasma Physics Laboratory code, Gkeyll, that was further developed to incorporate novel numerical development of a full nonlinear Fokker-Planck collision operator to model collisions accurately and efficiently.

Acknowledgment of Government Support and Government License

This work was generated with financial support from the U.S. Government through contract/Award No. DE-SC0018276, and as such the U.S. Government retains a paid-up, nonexclusive, irrevocable, worldwide

2 Major project goals

The major goals of the project were to enhance understanding of sheath physics and plasma-material interactions for regimes of relevance to tokamak disruption. More specific goals included incorporating interactions with neutrals and collisions towards more accurate theory and modeling of plasma transport in sheaths with a long-term goal of modeling sheaths in the presence of currents that flow between the plasma and the wall in tokamaks. An accurate sheath model is challenging when considering large plasma currents flowing into the wall along open field lines. The source of the current is due to a response to kink instabilities that result in a current on the outer edge of the plasma column. Addressing whether the current flows entirely into the wall or whether some of the current remains inside the plasma to complete the current loop without involving the wall remains an open research question. To enable this study, critical physics is necessary in the kinetic models to include elastic and inelastic collisions along with particle and power flow into the plasma domain to support modifications to sheath theory.

3 Progress towards accomplishing goals and summary of findings

This section provides a summary of research progress and key findings from this project.

3.1 Classical sheath studies with a wide range of Coulomb collisionality

Our contribution here was to derive an expression for the Bohm speed that is shown to be accurate over a wide range of plasma collisionality. Since the plasma is expected to be anisotropic in the sheath, the Bohm speed is derived from the transport equations of an anisotropic plasma. Particle-in-cell simulations verified the derivation to demonstrate the first predictive formula of the Bohm speed that has been shown to be quantitatively accurate over the intermediate plasma regime that is away from the asymptotic limit of vanishing Debye length and the limiting cases of adiabatic laws. Another key point of this work is that there is a sheath transition region that is spatially extended. Our analysis establishes the importance of an accurate plasma transport model in accounting for transport within the Knudsen layer next to the wall. To enable these contributions, we incorporated Monte Carlo collisions into the VPIC code, performed rigorous benchmarks, and applied the implementation towards this study. These results are summarized in the following peer-reviewed publications.

- Y. Li, B. Srinivasan, Y, Zhang, X.-Z. Tang, *Bohm criterion of plasma sheaths away from asymptotic limits.* Physical Review Letters **128**, 085002 (2022).
  Abstract: The plasma exit flow speed at the sheath entrance is constrained by the Bohm criterion. The so-called Bohm speed regulates the plasma particle and power exhaust fluxes to the wall, and it is commonly deployed as a boundary condition to exclude the sheath region in quasineutral plasma modeling. Here the Bohm criterion analysis is performed in the intermediate plasma regime away from the previously known limiting cases of adiabatic laws and the asymptotic limit of infinitesimal Debye length in a finite-size system, using the transport equations of an anisotropic plasma. The resulting Bohm speed has explicit dependence on local plasma heat flux, temperature isotropization, and thermal force. Comparison with kinetic simulations demonstrates its accuracy over the plasma-sheath transition region in which quasineutrality is weakly perturbed and the Bohm criterion applies.

- Y. Li, B. Srinivasan, Y, Zhang, X.-Z. Tang, *Transport physics dependence of Bohm speed in presheath-sheath transition.* Physics of Plasmas **29**, 113509 (2022).
  Abstract: The ion exit flow speed at the sheath entrance is constrained by the Bohm criterion, which is used as a boundary condition for simulations that do not resolve the sheath region. Traditional Bohm criterion analysis invokes the equation of state and, thus, ignores transport physics in the sheath transition problem. An expression for the Bohm speed away from the asymptotic limit is derived from a set of anisotropic plasma transport equations. The thermal force, collisional temperature isotropization, and heat flux enter into the evaluation of the Bohm speed. By comparison with kinetic simulation results, this expression is shown to be accurate in the presheath-sheath transition region rather than a single point at the sheath entrance over a broad range of collisionality.

Additionally, this work is also presented in the PhD dissertation of Yuzhi Li, who was funded on this award.

3.2 Applications to a plasma-sheath transition problem for a high recycling divertor in a fusion reactor

We implemented atomic collisions to model multiple reactions including ionization, recombination, charge exchange, and excitation in addition to elastic collisions with neutrals by extending the Monte Carlo collision module mentioned above to also incorporate collisions with neutrals in the code VPIC. This was necessary to extend the plasma sheath transition studies to the regimes of a high recycling divertor in a tokamak, where atomic collisions can significantly affect momentum and energy transport. Because neutrals concentrate near the wall due to the particle recycling process, ion-neutral collisions can produce a reduction in the ion exit flow speed. An expression for the Bohm speed is derived that accounts for anisotropic transport and the dominant atomic collisions in the sheath transition region. Our work shows that a tungsten wall versus a carbon wall in the divertor can produce different behavior with the carbon wall enhancing the neutral density and reducing ion temperature. Also, ion-neutral collisions are higher with carbon walls so the Bohm speed is reduced for carbon compared with tungsten. These are key contributions that can significantly impact material choices for tokamak divertors, including in the understanding and mitigation of disruptions. The results are summarized in the following peer-reviewed publication.

- Y. Li, B. Srinivasan, Y, Zhang, X.-Z. Tang, *The plasma-sheath transition and Bohm criterion in a high recycling divertor.* Physics of Plasmas **30**, 063505 (2023).
  Abstract: The high recycling regime of a divertor is characterized by high plasma particle fluxes and low temperature at the target, where a strong hydrogen recirculation loop exists. Atomic processes in the high recycling regime, such as ion-neutral friction and radiation, can affect the plasma momentum and energy transport in the sheath transition region. Here, the plasma-sheath transition near a high recycling wall is investigated. The Bohm speed, which constraints the ion exit flow speed, is evaluated from a transport model that accounts for the effect of the anisotropic transport and atomic collisions in the transition layer. A first principles kinetic code vector particle-in-cell with the atomic collision package is used to investigate a 1D self-consistent slab plasma with a high recycling boundary for the tungsten and carbon divertors. The results demonstrate the accuracy of the Bohm speed model in predicting the ion exit flow speed in the transition region, as well as the reduction of the Bohm speed due to the ion-neutral friction. The effect of different wall materials, tungsten, and carbon, on the Bohm speed and near-wall plasma profile is shown.

3.3 Using continuum-kinetic modeling to inform sheath boundary conditions

Kinetic simulations are necessary to accurately model microscopic phenomena that are critical to understanding plasma-material interactions and sheath physics. However, kinetic modeling remains infeasible for macroscopic modeling of tokamaks necessitating fluid modeling for global scales. Commonly used models for multi-fluid sheaths specify a flux at the walls assuming subsonic electrons and supersonic ions. The exact form of the flux specified is not clearly and accurately established. It is less clear how the sheath boundary conditions are modified to maintain accuracy when collisional physics and transport is taken into account, as summarized by the previously listed publications, and also for cases when magnetization can impact ion and electron flux to the wall. Our work uses continuum-kinetic sheath simulations of classical sheaths to inform multi-fluid modeling using equations and resolution aimed at resolving the sheath within the constraints of the assumptions of the moment model. We have shown that the Riemann problem, whether using an approximate or exact Riemann solver, provides a self-consistent boundary condition that allows resolution of the sheath within the constraints of the fluid model while allowing the flux to be determined by vacuum regions prescribed at the boundary. The comparisons of moments between the fluid and kinetic results produce excellent agreement. The results are summarized in the following peer-reviewed publication.

- P. Cagas, A.H. Hakim, B. Srinivasan, *A boundary value "reservoir problem" and boundary conditions for multi-moment multifluid simulations of sheaths.* Physics of Plasmas **30**, 063505 (2023).
  Abstract: Multifluid simulations of plasma sheaths are increasingly used to model a wide variety of problems in plasma physics ranging from global magnetospheric flows around celestial bodies to plasma-wall interactions in thrusters and fusion devices. For multifluid problems, accurate boundary conditions to model an absorbing wall that resolves a classical sheath remain an open research area. This work justifies the use of vacuum boundary conditions for absorbing walls to show comparable accuracy between a multifluid sheath and lower moments of a continuum-kinetic sheath.

3.4 Numerical algorithm development for the nonlinear Fokker-Planck collision operator in a continuum-kinetic model

Having demonstrated the importance of collisional modeling for plasma-material interaction and sheath physics for tokamak disruption simulations, we determined the need to develop and implement an accurate collisional model in the continuum-kinetic implementation as well. The continuum-kinetic code provides a noise-free framework within which one can model subtle sheath dynamics and instabilities that may not be discernible over PIC noise. Towards this, we developed and implemented a novel, fully-conservative, recovery-based discontinuous Galerkin (DG) algorithm for the full nonlinear Fokker-Planck collision operator using the Rosenbluth potential formulation. We developed a novel recovery scheme for the DG method that preserves high-order accuracy for the discretization of the diffusive flux of the surface terms, which is a tensor containing an accurate and efficient representation of the transverse derivatives of the distribution function in phase space without losing accuracy. While most nonlinear Fokker-Planck collision operators are computationally expensive, we have a novel implementation that is efficient, while maintaining accuracy and conservation of mass, momentum, and energy. This work is presented in the PhD dissertation of John Rodman, who was funded on this award for approximately the last year of his PhD where he completed the development and implementation of this collision operator continuing the work of Petr Cagas, who was a postdoc funded through this award. *Multiple manuscripts are in preparation for submission to peer-reviewed journals on the recovery-DG implementation of the high-order accurate, conservative, and efficient nonlinear Fokker-Planck collision operator.*

4 Training, professional development, career advancement

This award supported the PI (Bhuvana Srinivasan), a postdoctoral researcher and research scientist at Virginia Tech (Dr. Petr Cagas), PhD student (Dr. Yuzhi Li) full-time for the entire duration of his PhD, PhD student (John Rodman) full-time for the last year of his PhD, and PhD student (Kolter Bradshaw) for a short period during the early phase of his PhD. This award has contributed significantly to the career advancement of multiple individuals. Dr. Li defended his PhD in February 2023 and is presently a postdoctoral researcher at Los Alamos National Laboratory working with the lead-PI, Dr. Xianzhu Tang, of this SciDAC collaboration. John Rodman will be defending his PhD in November 2024 and hopes to continue working on problems of relevance to the DOE as a postdoctoral researcher. Dr. Bradshaw defended his PhD in January 2024 and is presently a postdoctoral researcher at Princeton University. Dr. Cagas is presently a research scientist with Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR).

5 Impact

5.1 Impact on principle discipline

When this work is complete, there is the potential for significant advances to be made both in modeling capabilities and the understanding of plasma- material interactions and Halo currents on tokamak disruption. The novel continuum kinetic modeling approach enables noise-free, high-dimensional kinetic simulations. We believe this modeling will have applications to a diverse set of plasma problems beyond magnetic fusion simulation. The particle-in-cell capabilities that we will be developing using the VPIC code and the long-term project goal of coupling to sophisticated collisional models such as FLYCHK will enable plasma sheath physics studies beyond the state- of-the-art.

5.2 Impact on other disciplines

The development of novel kinetic tools has applicability across a range of plasma physics applications from low-temperature to high-energy-density plasmas. The algorithm and model development that will be performed as a part of this proposal has broad applicability in applied mathematics and computational sciences as well.

5.3 Impact on technology transfer

The work produced by this grant will be published and the results will be made available to government funded entities such as researchers working on tokamak disruption in both the simulation and experimental domains. Further, the computational tools being developed will be made available to any interested parties.

5.4 Impact on society

Achieving controlled fusion has the potential to satisfy terrestrial energy needs for the foreseeable future. If results from this work provide a better understanding of tokamak disruption physics and disruption mitigation techniques, then they could contribute to the long-term development of fusion as an environmentally-friendly and economical energy source.

6 Products supported by this award

Journal Publications

[1] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “The plasma–sheath transition and Bohm criterion in a high recycling divertor”. In: *Physics of Plasmas* 30.6 (2023).

[2] Yanzeng Zhang, Yuzhi Li, Bhuvana Srinivasan, and Xian-Zhu Tang. “Resolving the mystery of electron perpendicular temperature spike in the plasma sheath”. In: *Physics of Plasmas* 30.3 (2023).

[3] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “Bohm criterion of plasma sheaths away from asymptotic limits”. In: *Physical Review Letters* 128.8 (2022), p. 085002.

[4] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “Transport physics dependence of Bohm speed in presheath–sheath transition”. In: *Physics of Plasmas* 29.11 (2022).

[5] Petr Cagas, Ammar H Hakim, and Bhuvana Srinivasan. “A boundary value “reservoir problem” and boundary conditions for multi-moment multifluid simulations of sheaths”. In: *Physics of Plasmas* 28.1 (2021).

Theses & Dissertations

[1] Yuzhi Li. “The Effects of Collisions on Plasma-Sheath Transition”. Virginia Tech, Ph.D. dissertation, 2023.

[2] John Rodman. “Discontinuous Galerkin Studies of Collisional Dynamics in Continuum-Kinetic Plasma”. Virginia Tech, Ph.D. dissertation, expected 2024.

Presentations

[1] John Rodman, James Juno, and Bhuvana Srinivasan. “Discontinuous Galerkin simulations of the nonlinear Rosenbluth/Fokker-Planck collision operator”. In: *APS Division of Plasma Physics*. APS, 2024.

[2] John Rodman, James Juno, and Bhuvana Srinivasan. “A recovery-based discontinuous Galerkin scheme for the Fokker-Planck collision operator”. In: *APS Division of Plasma Physics*. 2023.

[3] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “Bohm criterion of plasma sheaths away from asymptotic limits”. In: *APS Division of Plasma Physics* Invited Talk. 2022.

[4] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “Bohm criterion of plasma sheaths away from asymptotic limits”. In: *Sherwood Fusion Theory Conference* Invited Talk. 2022.

[5] Petr Cagas, Ammar Hakim, and Bhuvana Srinivasan. “A recovery-based numerical scheme for full Fokker-Planck collisions”. In: *APS Division of Plasma Physics*. 2021.

[6] Yuzhi Li, Bhuvana Srinivasan, Yanzeng Zhang, and Xian-Zhu Tang. “The influence of atomic collisions on the sheath profile”. In: *APS Division of Plasma Physics*. 2021.

[7] Petr Cagas, Ammar Hakim, and Bhuvana Srinivasan. “Studies of plasma sheaths using novel numerical schemes with self-consistent emitting walls and full Fokker-Planck collisions”. In: *APS Division of Plasma Physics* Invited Talk. 2020.

[8] Yuzhi Li, Bhuvana Srinivasan, and Xian-Zhu Tang. “The effect of a collisional presheath on the Bohm criterion”. In: *APS Division of Plasma Physics*. 2020.

[9] Petr Cagas, Ammar Hakim, Jimmy Juno, and Bhuvana Srinivasan. “Conservative Recovery Discontinuous Galerkin Scheme for the Fokker-Planck Collision Operator”. In: *APS Division of Plasmas Physics*. 2019.

[10] Yuzhi Li, Bhuvana Srinivasan, Xian-Zhu Tang, and Jun Li. “Influence of collisions on sheath profile”. In: *APS Division of Plasma Physics*. 2019.

[11] Kolter Bradshaw and Bhuvana Srinivasan. “Continuum kinetic simulations of the Weibel instability in plasma sheaths”. In: *APS Division of Plasma Physics*. 2019.

[12] Bhuvana Srinivasan, Petr Cagas, Ammar Hakim, Yuzhi Li, Jun Li, and Xian-Zhu Tang. “Kinetic simulations of wall-bounded plasmas”. In: *International Conference on the Numerical Simulation of Plasmas*. 2019.

[13] Petr Cagas, Bhuvana Srinivasan, and Ammar Hakim. “High-order Discontinuous Galerkin Discretization for Multi-physics Simulations of Plasmas”. In: *SIAM CSE miniconference* Invited Talk. 2019.

[14] Yuzhi Li, Bhuvana Srinivasan, Xian-Zhu Tang, and Zehua Guo. “Kinetic studies of sheaths at tokamak edge”. In: *APS Division of Plasma Physics*. 2018.