NORTH ATLANTIC TREATY ORGANIZATION

SCIENCE AND TECHNOLOGY ORGANIZATION

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STO TECHNICAL REPORT **TR-AVT-294**

Towards Improved Computational Tools for Electric Propulsion

(Vers des outils de calcul améliorés pour la propulsion électrique)

Final report for NATO AVT-294 RTG.

Published August 2022

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The NATO Science and Technology Organization

Science & Technology (S&T) in the NATO context is defined as the selective and rigorous generation and application of state-of-the-art, validated knowledge for defence and security purposes. S&T activities embrace scientific research, technology development, transition, application and field-testing, experimentation and a range of related scientific activities that include systems engineering, operational research and analysis, synthesis, integration and validation of knowledge derived through the scientific method.

In NATO, S&T is addressed using different business models, namely a collaborative business model where NATO provides a forum where NATO Nations and partner Nations elect to use their national resources to define, conduct and promote cooperative research and information exchange, and secondly an in-house delivery business model where S&T activities are conducted in a NATO dedicated executive body, having its own personnel, capabilities and infrastructure.

The mission of the NATO Science & Technology Organization (STO) is to help position the Nations' and NATO's S&T investments as a strategic enabler of the knowledge and technology advantage for the defence and security posture of NATO Nations and partner Nations, by conducting and promoting S&T activities that augment and leverage the capabilities and programmes of the Alliance, of the NATO Nations and the partner Nations, in support of NATO's objectives, and contributing to NATO's ability to enable and influence security and defence related capability development and threat mitigation in NATO Nations and partner Nations, in accordance with NATO policies.

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- AVT Applied Vehicle Technology Panel
- HFM Human Factors and Medicine Panel
- IST Information Systems Technology Panel
- NMSG NATO Modelling and Simulation Group
- SAS System Analysis and Studies Panel
- SCI Systems Concepts and Integration Panel
- SET Sensors and Electronics Technology Panel

These Panels and Group are the power-house of the collaborative model and are made up of national representatives as well as recognised world-class scientists, engineers and information specialists. In addition to providing critical technical oversight, they also provide a communication link to military users and other NATO bodies.

The scientific and technological work is carried out by Technical Teams, created under one or more of these eight bodies, for specific research activities which have a defined duration. These research activities can take a variety of forms, including Task Groups, Workshops, Symposia, Specialists' Meetings, Lecture Series and Technical Courses.

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Towards Improved Computational Tools for Electric Propulsion

(STO-TR-AVT-294)

Executive Summary

This document provides a summary of the activities of the NATO AVT-294 RTG. After a brief overview of the importance of computational tools for EP to accelerating the transition of plasma thruster technology, the bulk of this work focuses on new areas of emphasis which should be pursued with particular focus on synergies with larger emerging technological trends including massively parallel computing and machine learning. The document also provides a series of recommendations to assist decision makers in targeting additional investment areas to maximize benefit of computational tools for EP to advancing NATO space capabilities.

Vers des outils de calcul améliorés pour la propulsion électrique

(STO-TR-AVT-294)

Synthèse

Le présent document fournit un résumé des activités du RTG AVT-294 de l'OTAN. Après une brève présentation générale de l'importance des outils de calcul pour la propulsion électrique, dans l'optique d'accélérer la transition de la technologie des propulseurs à plasma, ce document se concentre principalement sur les nouveaux domaines à étudier, notamment sur les synergies avec les tendances technologiques émergentes de plus grande ampleur, incluant le calcul massivement parallèle et l'apprentissage automatique. Le document contient également une série de recommandations pour aider les décideurs à cibler d'autres domaines d'investissement et optimiser le bénéfice des outils de calcul pour faire progresser les capacités spatiales de l'OTAN à travers la propulsion électrique.

TOWARDS IMPROVED COMPUTATIONAL TOOLS FOR ELECTRIC PROPULSION

1.0 INTRODUCTION

The NATO AVT-294 RTG effort was established to assess and improve NATO member coordination in computational activities supporting Electric Propulsion (EP). In part, this reflects the degree to which EP is acknowledged as an enabling propulsion technology for critical NATO space assets; however, it also reflects the degree to which improvements in computational tools will be critical to driving down the high cost (both performance and schedule) of the actual development, deployment, and optimization of these high performance propulsion systems.

The structure of this document is as follows. In Section 2.0, major obstacles to the effective transition of EP devices to operational spacecraft design are discussed. Next, in Section 3.0, a discussion is provided to highlight particular complexities of EP thruster physics which make numerical simulation modeling so challenging. Section 4.0 provides a short introduction to the state and taxonomy of existing EP computational tools. The core of this document is contained in Section 5.0, which addresses overarching technological trends and their relationship to the future of improved computational tools for EP. Finally, Section 6.0 summaries the principal recommendations emerging from this effort.

2.0 OBSTACLES TO TRANSITION

EP devices offer significant performance advantages versus chemical propulsion. The chief advantage is the high efficiency with which they are able to use propellant, as measured by the specific impulse. For instance, compared to in-space chemical propulsion alternatives running at 220 s (hydrazine monopropellants) and 330 s (MMH-NTO bipropellants), common EP specific impulses range from 1500s – 2500s (HETs) to 2000s – 3000s (Ion Engines), indicating almost a 10x lower propellant burn rate to achieve the same thrust level.

Unfortunately, due to fundamental constraints of reaction engines which produce thrust via momentum transfer to exhaust particles, the Thrust to Power (T/P) of an EP device scales inversely with the specific impulse. Therefore, unless one is able to provide large amounts of electric power, the necessary consequence of an EP thruster with very high ISP is very low thrust. Given finite power available on-orbit (typically from solar panels), this means that a significant change in the spacecraft velocity vector (delta-V) requires operation of the thruster for sustained periods of time. It is not uncommon for EP thrusters to be operated for tens to hundreds of hours at a time and typically HET thruster lifetimes are measured in thousands of hours. This is in comparison to chemical thrusters, which may have thruster lifetimes of only minutes at the 100 N+ thrust level. An excellent reference for basic in-space propulsion systems can be found in Ref. [1].

This foundational characteristic of EP operation – the need to operate for thousands of hours – leads to the biggest transition obstacle, namely the high cost and significant time required to meet Mission Assurance (MA) needs. Parsing MA further, multiple transition challenges include the:

- **High cost of long-duration ground testing** – Vacuum chambers are fairly expensive to build and operate. Given that thousands of hours are required for lifetime tests, this is not only a significant direct expense but also reduces availability for development activities.

- **Reduced fidelity of the ground test environment** – It is well known that even the largest vacuum chambers with millions of liters/second of pumping speed cannot match the pressure environment of space, particularly for 10+ kW thrusters. In addition, plume interactions with the chamber walls can lead to thruster contamination concerns which are not representative of the space environment, particularly in the context of realistic space weather. Finally, the plasma produced by EP devices shares electrical information with the chamber walls through coupled sheath physics, leading to interaction potential between the thruster and vacuum chamber.

The development of a virtual plasma simulation environment encompassing both EP thruster and their environment offers a promising strategy to address all these MA challenges. Moreover, the ability of numerical tools to rapidly simulate arbitrary geometries and boundary conditions for both the thruster and chamber (or lack thereof) also has the potential to dramatically accelerate new EP thruster development and optimization. Furthermore, future integration of propulsion into more complex systems (i.e., satellites and even entire space architectures) must adapt to a larger industry trend towards Digital Engineering [2]. At present this has already prompted the widespread use of digital artifact generation across all phases of design and test, from mechanical/structural design and thermal design all the way to qualification testing. However, computational tools for EP thrusters are not fully engaged in this process, largely due to the lack of maturity in computational tools. In large part, this is due to the physical complexity of real-world EP devices covered in the next section.

3.0 COMPLEXITY OF EP THRUSTER PHYSICS AND OPERATION

There are multiple levels at which to understand the complexity of EP thruster physics. An excellent text to understand the design and operation of EP thrusters can be found in Ref. [3]. This level of conceptual understanding, combined with experimental testing and traditional probe-based plasma diagnostics, provide practical and quantifiable inputs to modern EP thruster maturation efforts. However, a deeper level of understanding is stymied by the fundamental complexity of real-world EP systems. In particular the strongly coupled nonlocal interaction of nature of plasma via electromagnetism, non-ideal characteristics of magnetic and physical confinement, and the absence of strong, fast collisional relaxation processes leads to a classical multiscale/multiphysics situation. Recent discussion of progress across a large range of canonical ExB physics challenges for EP can be found in Ref. [4].

The crux of EP thruster complexity comes from the dynamic response of the plasma configuration as it is accelerated by electromagnetic/electrostatic forces to generate thrust. At an engineering level, this interaction with electrical forces is often conceptualized as a bulk force acting on a “passive” unit plasma volume; however, some amount of plasma reconfiguration (such as a change in the velocity distribution function or energy/momentum loss to ionization) occurs within the unit plasma volume. This process is also strongly modulated by the presence of plasma waves, and coherent interactions between particles through electromagnetic and collisional couplings in the bulk fluid. A century of effort from the plasma physics community has established rigorous theoretical models for plasma waves, addressing both fluid and kinetic plasma descriptions and including quantitative metrics for onset of wave growth and estimates for nonlinear saturation values. Yet despite these efforts, multiple gaps still exist in our ability to apply this theory to EP devices including:

Insufficient dimensionality – theoretical investigation typically focuses on reduced dimensional analysis (often 0D spatially and only 2D in velocity); non-optimal real-world effects reducing performance and leading to thruster degradation exist in a true 3D3V[1] (footnote: 3 space dims, 3 velocity dims) context. → **Computational tools must address high dimensional simulation**.

[1] ExB physics refer to plasma transport in configurations with orthogonal electric and magnetic field components. Classical collision-based theoretical prediction dramatically underestimates observed ExB transport rates. These enhanced ExB transport rates are a primary cause for reduced efficiency of many magnetic confinement devices.

Little to no coupling (momentum and energy transfer) between different types of plasma waves – for reasons of computational tractability, plasma theory typically focuses only a single canonical wave structure (planar, helical, etc.) at a time. Moreover, response times due to electromagnetic interactions (measure in fractions of the speed of light) mean that wave growth responds extremely quickly to changes in the plasma state. Therefore, any changes in the plasma configuration can readily influence information exchange between waves. These internal nonlinear couplings, combined with other known interactions, contribute to the incredibly interesting phenomena of both mode transitions [5] and hysteresis in HET operation. → **Computational tools must address these coupling either through direct simulation or models which incorporate potential nonlinear crosstalk between wave modes**.

Spatiotemporal plasma non-uniformity – multiple orders of variation in fundamental plasma characteristics means that EP thrusters can simultaneously support different plasma waves across space and time. Relevant plasma length scales vary from meters (size of chambers) to 10 s of microns (Debye length) while relevant timescales vary from years (total thruster lifetime) all the way to nanoseconds (plasma frequency). An excellent review of relevant plasma waves present in HET plasmas can be found in Ref. [6]. Moreover, interactions with physical surfaces in wall bounded plasmas leads to significant anisotropy in velocity space, further increasing the complexity of the plasma description. → **Computational tools must address an enormous range of time and length scales**.

Beyond these core plasma challenges, numerous other aspects of complexity exist throughout the EP field. Highlights of these challenges include:

Spacecraft Integration – Certain EP systems are known to have potential integration impacts due to non-negligible fractions of energetic plasma which intersects with the space vehicle itself. This interaction, called sputtering, can remove anti-reflective coatings, multi-layer insulating blankets, and, given sufficient time, virtually any spacecraft components within the line-of-sight of the thruster. As spacecraft components are sputtered away, they now have a new potential for re-deposition: to drift to regions beyond line-of-sight of the thruster and redeposit on cold spacecraft surfaces, including on solar panels and sensor lenses. In addition, the presence of bulk plasma can adversely affect EM transmission from RF payloads and modify the spacecraft charging environment. → **Computational tools must address the interactions between plasma and a huge variety of potential surfaces and describe the plasma evolution far beyond the thruster exit plane**.

Space Weather – whether a spacecraft is designed for military or scientific utility, it exists in the very harsh environment of space. Therefore, the understanding of the stochastic properties of the space environment, including the frequency and duration of solar storms, is a strong driver in spacecraft design. Moreover, a fundamental need to understand the plasma environment exists from a military perspective. For instance, in a situation where a flight CPU malfunctions, it is absolutely critical to understand whether it is a function of statistically rare but naturally occurring phenomena or the result of interaction with an artificial environment. Therefore, whether the plasma environment is due to natural fluctuations or is artificially manipulated through the local operation of EP devices, improved models for these effects are of great interest to both the design and operation of spacecraft. → **Computational tools must propagate the effects of the plasma environment onto the spacecraft internal structure and functionality**.

Electric Configuration – Between spacecraft charging and PPU design, the coupling between reactive/resistive behavior of the thruster, the spacecraft, and the local environment all play a role in effective operation. Moreover, cathode behavior, while often reduced to an idea current source, are an integral part of the electrical circuit and thus have a major role in thruster performance and stability. → **Computational tools must incorporate electric coupling effects and related engineering design with high enough confidence for acceptable integration risk**.

Beyond these concerns, effective development of new EP devices will face levels of difficulty in many additional areas not addressed here. For instance, exciting new futures for air-breathing or In-Situ Resource Utilization (ISRU) will introduce the additional complexity of molecular and polyatomic plasmas and increased interest in very high power yet throttleable EP systems dramatically increase interest in pulsed EP systems. There is very little debate that significant new capabilities for EP computational tools are required to meet pressing future challenges.

4.0 STATE OF COMPUTATIONAL TOOLS

Computational tools in EP have existed for almost as long as EP has existed as a field. The diversity of EP thruster technologies represents a huge span in different plasma conditions, prompting very different choices in underlying model descriptions (both for the bulk fluid and ancillary physics) and discretization. Covering the depth and breadth of progress across the field is beyond the scope of this report (although excellent references can be found in recent reviews [7], [8]). Critically, though, there are two major discriminators in intended application which can be used to distinguish many of these efforts.

- *Thruster Codes* versus *Spacecraft Integration Codes* – There is a fairly clear distinction between plasma thruster codes, which typically encompass a computational volume with characteristic dimensions on the same order as the thruster, versus spacecraft Integration codes, which include not only the thruster(s) but also the spacecraft and/or local environment and typically encompass a computational volume with characteristic dimensions of the spacecraft. While one-way coupling from thruster codes into integration codes have been attempted [9], there has not yet been demonstrated a robust coupling (i.e., two-way information flow) between a thruster and spacecraft integration codes. Examples of common engineering codes include HPHall [10], Hall2De [11] and many others [12], [13] and examples of common spacecraft integration codes include COLISEUM [14], TURF [15], and SPIS [16].
- *Science Codes* versus *Engineering Codes* – The distinction between these two types of efforts is considerably less distinct. Science codes typically attempt more ambitious (greater spatiotemporal resolution) simulations with less emphasis on resolving the true dimensionality or physical configuration (dimensions/materials) of actual EP devices. Engineering codes typically trade lower spatiotemporal resolution and significant use of subgrid scale models to describe under-resolved physics, for the ability to capture realistic geometries (potentially including chamber boundaries) with fairly short run-times.

Theoretically, increased computational resources combined with more sophisticated software implementations reduce these distinctions and have the potential to provide an overarching computational capability (the virtual space plasma simulator) spanning these discriminators. However, in practice, due to the enormous challenges identified in Section 2.0, evolutionary progress will likely continue be made on a discrete subset of these discriminators. Advantageous alignment of larger technological trends with existing R&D trends in the EP community, discussed in the next section, offer a potential avenue to accelerate this progress.

5.0 EMERGING CHALLENGES AND OPPORTUNITIES

This section contains the core findings of this document organized into three main themes. First, a discussion is provided on the impact of High Performance Computing (HPC) and future possible impact as applied to EP simulation. Second, algorithmic strategies to promote automated exploit strategies for the vast quantities of data from HPC are discussed. Third, a brief discussion is provided on potential for data assimilation opportunities to facilitate the synchronization of M&S with physical systems.

5.1 High Performance Computing

While past decades have seen an enormous increase in raw processing power (as measured in FLOPs), equally important to HPC is the increasing maturity of sophisticated scientific computing frameworks to facilitate the study of plasma configurations relevant to EP. Particularly for Hall Effect Thruster (HET) simulation, which requires the solution of Poisson's equation, the availability of fast multigrid parabolic solvers such as HYPRE [17] have had an enormous impact on the ability to effectively leverage massive computer assets to resolve coupled electron kinetics/field behavior at meaningful Debye length and plasma frequency scales. Thus, there is now a dramatically increased number of powerful science codes available to study particle-wave instabilities, particularly the Electron-Drift Instabilities (EDIs) believed to drive a significant fraction of electron transport. In addition, even modest computational clusters now provide sufficient computational resources to handle high dimensional problems – for instance, capabilities exist for 2D2V [18], [19], 3D3V PIC [20] and even 2D3V Vlasov plasma simulation [21] of HETs with engineering codes. In addition, for ancillary physics such as wall-plasma integration, the introduction of Molecular Dynamics (MD) models to study microscale processes in erosion and sputtering have allowed for the extension of macroscale sputtering models to considerably lower impact energies than is possible experimentally [22].

Nevertheless, there remain a number of challenges in HPC deployment. First, scientific computing still faces a tradeoff between code scalability and extensibility. For instance, the allure of the raw arithmetic calculation power of new hardware architectures, particularly heterogeneous architectures, is somewhat diminished by the need to optimize data transfer for relatively high latency communications between General Purpose Graphical Processing Units (GPGPUs). This complication requires specialized algorithm development which slows deployment of new capabilities, particularly with the addition of additional physics modules, which require data transport paths that do not fit the same paradigm as the original plasma simulation framework. The challenges of incorporating complex collision physics, geometric complex wall interaction models, and potentially even radiation or dynamic thermal effects further increases the complexity of this software development effort.

A parallel challenge exists in the application of scientific codes (largely using HPC) to engineering devices. In addition to the multiphysics challenges referred to above, there is also a multiscale problem. To some extent, advances in algorithms, such as high performance Implicit PIC such as iPIC3D [23], can effectively address many of the temporal challenges. However, there are still requirements to resolve fundamental spatial scales which put an effective floor on speedup potential. In the long term, pursuing true two-way coupling between thruster and integration codes will likely require the further adoption of a broad range of multiscale simulation techniques to simulate all the way from the thruster throughout the entire spacecraft domain.

The opportunities that HPC have provided to the EP simulation community are vast – they unlock a vast and powerful new "virtual" test capability which can model the evolution of instabilities all the way from linear growth through nonlinear saturation in truly 3D, rather than reduced dimensional contexts. Moreover, unlike experimental test campaigns, the output of these simulations is accessible to micron lengths and nanosecond accuracy without the limitations of probe or spectroscopic theory. This ability of HPC to provide vast, detailed datasets also provides a huge challenge for interpretation – the sheer volume of data generated prohibits purely human interpretation. Fortunately, significant advances are occurring in the field of automated data exploitation.

5.2 Dataset Exploitation

HPC-level plasma simulation provides a uniquely instrumented environment to explore the evolution of coherent plasma structure through the complex set of nonlinear interactions encoded in the coupling between Maxwell's equations and Boltzmann's equation. However, it is incredibly resources intensive and thus will not be available as a responsive design tool tightly integrated into thruster design iterations. This leads to a critical challenge – distilling the output of vast numerical (or even experimental) datasets into concise mathematical forms for engineering codes. HPC dataset exploitation is a clear companion to increased HPC deployment – many efforts are already active in this area are active, including promising work by Lafleur [24] in deriving transport coefficients for fluid codes from kinetic simulation. The focus of the following subsections is on broad algorithmic advances which have the potential to automate significant portions of dataset exploitation. These include:

- **Reduced Order Models (ROMs)** – The promise of ROMs is the discovery of vastly lower dimensional subspaces which approximately but accurately represent the full dimensional (i.e., all values at all grid points over all simulation time) plasma configuration. An analogue from signal processing is the following – imagine a discrete digital representation of an audio signal, transformed to the frequency domain using the FFT – a ROM for this system might represent the subset of Fourier modes which represent the highest 95% of the signal power. Popular ROM strategies include Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD), both of which can be readily applied to massive multidimensional plasma simulation outputs to identify optimal bases and compactly represent the spatiotemporal evolution of coherent structures. These new bases can be folded back into the original systems of coupled PDEs to formulate a reduced set of coupled equations or can serve as the basis for data-driven simulation strategies. The complexity of nonlinear plasma evolution remains a challenge for robust projective ROM discovery, but early progress is underway in EP [25] and a significantly more mature effort is demonstrating good progress in accelerating simulations of liquid rocket engine combustion [26], [27]. Note that other reduced order modeling strategies apply to many other EP relevant physics, including recent work in collisional-radiative mechanism reduction for EP plasmas [28].
- **Model Discovery via Machine Learning (ML)** – Despite the incredible success of plasma theory in explaining a host of observed EP phenomena, real-world effects (distribution function anisotropies, collisional behavior, and non-ideal wave structures) and the often nonlinear evolution of coherent structures mean that models developed with microscale intuition often lose accuracy when utilized in meso/macroscale resolution in engineering codes. For example, electron fluid models popularly used in HET engineering codes rely heavily on subgrid scale models for enhanced electron transport (so-called anomalous transport) to accurately capture macroscopic electron motion. Microscale plasma theory, such as Bohm turbulence [29], near-wall conductivity [30], EDI [31], [32], [33], and even entropy arguments [34], have been used to justify the functional form of subgrid scale models for enhanced electron transport. Despite rigorous theoretical underpinnings of these models, real-world effects diminish the accuracy of these models and significant model calibration is required to simulate realistic thruster performance. In an era of data-driven discovery, new techniques for automated model discovery, as recently demonstrated by Jorns [35], have demonstrated the feasibility of using Machine Learning techniques to identify relevant functional forms for new candidate subgrid scale models for enhanced electron transport.

It should be noted that while tools for both ROM and ML are readily applicable to the enormous datasets generated to HPC datasets, they are fundamentally data-driven discovery methods. For this reason, they should be considered as a complement, and not a replacement, for existing theory-based analysis. This is because the accuracy of data-driven methods hinges on the quality and relevance of input datasets. A subgrid scale transport model trained in one operating regime may be significantly less accurate in other thruster operating regimes – completely data-driven approaches, absent an overarching physics framework, have reduced applicability for generalized predictive use away from the training data. It should be noted that traditional plasma theory has related, but far more well understood, set of limitations – often captured via asymptotic limits such as high

Knudsen numbers or small Hall parameters. Therefore, assessing the validity of any approximate numerical prediction, whether based on a ROM or hybridization of physics-based and data-based/theory-based models in an engineering code, warrants the application of rigorous Validation Verification and Uncertainty Quantification (VVUQ) strategies discussed in the next section.

5.3 VVUQ and Data Assimilation

The ultimate goal of computational tools in EP is to drive down obstacles to the development and transition of real-world devices in the space environment. This has three major implications discussed in this subsection. First, the relationship between even high-resolution plasma models and physical devices is rarely truly one-to-one (e.g., numerical constraints drive mathematical approximations and manufacturability constraints lead to geometric non-uniformities). This means that a growing emphasis on Uncertainty Quantification (UQ) is recognized as a prerequisite for more useful application of numerical tools to EP thruster design and MA. Second, the Verification and Validation (V&V) of EP thrusters, particularly for engineering codes, is greatly complicated by nonlinear interactions between differing numerical implementations, subgrid scale physics models, and the sheer difficulty in making accurate, repeatable measurements in dynamically varying, low-density plasmas. Third, and finally, the relationship between numerical codes and physical systems for dynamically evolving systems is sufficiently complex that complimentary strategies for data assimilation should be investigated as a strategy to further synchronize plasma simulations to physical systems.

- **Uncertainty Quantification** – At a very basic level, UQ represents a set of strategies to understand the nonlinear sensitivities of outputs to variations in input parameters. Given the omnipresence of uncertainty in both simulation (discretization error, model approximations) and the real-world (measurement error, probe theory approximations), UQ will necessarily become a larger focus in EP as computational products move from qualitative to quantitative inputs for thruster design. Early efforts by Jorns [36] represent a critical acknowledgement that the output of thruster lifetime simulations for imperfect real-world devices should be statistical measures of confidence rather than the absolute certainty of a single deterministic outcome. Similarly, the role of measurement uncertainty in subgrid scale model development must also be considered – recent work by Yim [37] demonstrates the application of Bayesian inference tool subgrid scale physics model development. This idea of unavoidable uncertainty can be extended yet further into improved validation for entire computational codes. While HET engineering codes can be successfully calibrated very closely to experimental measurements, assessing the robustness of these calibrated predictions to perturbations in real-world geometries and operating conditions using UQ techniques will provide greater confidence in erosion predictions and lifetime assessment.
- **Verification and Validation (V&V)** – V&V has historically been robustly explored in both the plasma and CFD communities through traditional methods such as grid convergence in the context of the method of manufactured solutions (verification) and comparison with accepted basic plasma theory (validation). The challenges of V&V in an EP thruster context are hugely complicated by the almost omnipresent dynamical coupling of multiphysics effects in these devices. For this reason, it is not sufficient to simply perform V&V on individual physics modules and expect a combination of those modules to demonstrate similar levels of accuracy. The nonlinearity of thruster physics – a complex balance between energy flows into and out of the plasma – is well recognized and major efforts are underway to address V&V of these devices. A recent large-scale code verification collaboration [38] in the context of the larger LANDMARK validation project [39] is directly addressing high permutations of V&V through different couplings of integrators, field solvers across multiple dimensions. These community-wide efforts mirror similar maturation trajectories in other plasma communities, including magnetic reconnection [40] and partially magnetized plasmas [41]. In addition,

considering of HET behavior through the lens of dynamical systems theory offers the potential for new V&V metrics well-suited to high-speed measurements readily available from many common experimental diagnostics [42].

- **Data Assimilation** – The use of experimental data to calibrate subgrid scale models for electron transport is a common practice for effective use of engineering HET codes today. Although the trajectory of HPC simulation does point towards a future capability for truly predictive thruster simulations off engineering codes, the computational cost will still be immense and rigorous UQ will not be possible on such expensive simulations. Especially in a thruster design context, therefore, the integration of experimental data into M&S codes represents a complementary avenue to different data exploitation strategies. For example, injecting appropriate sensor data into even an approximate model can effectively synchronizes the simulation with real-world dynamics. An early attempt at the application of Kalman filtering to neutral dynamics by Greve [43] has demonstrated the utility of a single experimental data stream to anchor the time evolution of a complex nonlinear code. While data assimilation is still a fairly nascent research area in the EP community, it offers an intriguing possibility to leverage the explosion in the availability of data (thanks to low-cost sensors and DAQ systems) to develop lightweight Digital Twins [44] to complement heavyweight HPC simulation capabilities.

Opportunities in this area are of particular interest because of the focus they place on tighter coordination between computational and experimental disciplines. Whether explicitly (UQ) or implicitly (V&V, data assimilation), these opportunities require objective evaluation of the confidence which should be realistically placed in observable data streams – whether derived virtually or from physical sensors – reflect the true state of the system. The challenge of this question ties strongly to the fundamental challenge of Mission Assurance and the need for greater confidence that computational tools can be used as effective representations of real-world systems.

6.0 SUMMARY AND RECOMMENDATIONS[2]

The distinct area of [Electric Propulsion] basic plasma physics has been relatively poorly explored and is not well understood, but is within reach of current analytical and numerical capabilities, as well as powerful modern diagnostic tools.

– *Jean-Pierre Boeuf,* [45].

The simple promise of computational tools in EP is the ability to harness the horsepower of computers to extend physics theory to domains of real relevance to practical thruster systems. Relentless capability growth in HPC hardware, coupled with the maturation of scientific computing libraries, offer new opportunities to access this predictive power to simulate the complex dynamical behavior of plasma thrusters. However, in the context of computational tool development for EP, additional physics (such as collisional effects, power supply models, and wall conditions) remain to be incorporated.

Recommendation 1:

- Continue evolution of cutting-edge HPC tools (including incorporation of multiphysics effects) to generate a library of true 3D/3V canonical thruster simulations.

[2] Note that the recommendations provided represent a summary within the limited scope of this activity. It should not be considered as comprehensive within the computational space, nor is it intended to supersede existing experimental and theoretical R&D efforts.

- Continue leverage/development of multiscale algorithms to extend HPC simulation capabilities to even larger spacecraft-scale domain while retaining appropriate resolution inside thruster.

The increased availability of enormous data streams, both numerical and experimental, pose an exciting new opportunities to leverage advanced in automated data exploitation to accelerate computational tool development. At the crux of these activities are a host of data exploitation strategies to generate approximate lower dimensional models and bases for fast, yet accurate engineering codes. As data-driven techniques, application of these techniques exists primarily as an interpolative acceleration mechanism.

Recommendation 2:

- Significantly enhance the emphasis on exploitation of automated data exploitation techniques to complement canonical thruster simulations.

Increased application of computational tools to real-world problems requires increased investment into the maturing area of VVUQ. The EP community has already demonstrated strong collective interest in this area, although the complexity and nonlinearity of plasma interactions will pose significant challenges beyond simplified grid convergence analysis. Application of data assimilation techniques – the logical extension to well-accepted model calibration activities – may offer solutions to resolving the fundamental tradeoff between of resolution and responsive computational simulation through periodic state synchronization between codes and real systems.

Recommendation 3:

- Support expanded emphasis on community-wide code verification and validation activities
- Exploration of potential roles for data assimilation R&D efforts into existing numerical activities

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14. Abstract

This document provides a summary of the activities of the NATO AVT-294 RTG. After a brief overview of the importance of computational tools for EP to accelerating the transition of plasma thruster technology, the bulk of this work focuses on new areas of emphasis which should be pursued with particular focus on synergies with larger emerging technological trends including massively parallel computing and machine learning. The document also provides a series of recommendations to assist decision makers in targeting additional investment areas to maximize benefit of computational tools for EP to advancing NATO space capabilities.

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