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TRANSP Workshop Summary
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Introduction

The TRANSP Code Workshop provided a platform for in-depth discussions on advancing the capabilities of the TRANSP code [1, 2, 3], focusing on key areas such as predictive capabilities, interpretive frameworks, core-edge coupling, and integration with engineering components. More than 25 scientists from PPPL and around the world contributed to the workshop by making presentations and participating in discussions.

The workshop covered a range of topics including:

- **Current Status of TRANSP:** Discussions focused on the present state of TRANSP, encompassing assessments of the current code infrastructure, the dynamics of the user base, and the existing support mechanisms.
- **Code Infrastructure, Core-Edge Coupling, and Engineering Integration:** Efforts were made to address the enhancement of the code infrastructure, including improvements in interfaces and the integration of engineering components into the TRANSP code. This approach aimed at refining the code's technical aspects and expanding its applicability into engineering-related applications.
- **Enhancing Interpretive Capabilities:** Participants discussed the importance of advancing interpretive capabilities, specifically focusing on improving the analysis of experimental data and enhancing model validation processes.
- **Predictive Capabilities for Discharge Optimization:** Considerable attention was directed towards the evolving needs in predictive capabilities, particularly concerning their application in discharge optimization, planning, and the design activities associated with Fusion Power Plant (FPP). The discussions aimed at aligning TRANSP with the evolving demands of forward-looking fusion research.

These comprehensive discussions emphasized the workshop's commitment to diverse aspects of TRANSP, from its foundational elements and user-oriented dynamics to its evolving roles in both interpretive and predictive analysis. This ensures its relevance and effectiveness in the developing landscape of fusion research.

1. Current Status of TRANSP and User Support

The current status of the TRANSP code was described in the presentations by Alexei Pankin (PPPL). He highlighted that with almost 300 researchers from 30 institutions registered at the PPPL cluster, a notable increase in TRANSP runs throughout 2023 was recorded. The first eight months of the year have already seen a remarkable surge, with the total number of runs experiencing an approximate 50% uptick compared to the same period in 2022. Specifically, the overall number of runs escalated from 4864 (with 3832 executed in parallel) to 7276 (with 4402 executed in parallel). This surge in activity reflects a vibrant and expanding community of researchers using TRANSP for their studies and analyses.

The latter portion of Pankin's presentation centered around ongoing TRANSP development projects, notably highlighting a significant initiative focused on integrating IMAS interfaces into TRANSP. This development project aims to establish a cohesive framework for accessing both experimental and modeling data uniformly, facilitating seamless coupling with external modules that align with IMAS standards, thereby enhancing the interoperability and versatility of TRANSP. Alexei also introduced several ideas for prospective code development projects, providing insight into how TRANSP will evolve in the future.

User support needs were described in a presentation by Marina Gorelenkova. Through an analysis of various statistical data pertaining to TRANSP runs, she highlighted a rise in the demands for user support. The presentation also addressed the existing methods for user interaction, which are currently facilitated through the TRANSPHub repository on GitHub, regular open office hours held weekly, and monthly meetings involving representatives from collaborative research organizations. These channels serve as integral mechanisms for providing support, fostering collaboration, and addressing the evolving needs of TRANSP users.

The current TRANSP code infrastructure was presented by Jai Sachdev. Jai delivered an analysis centered on the self-assessment of software metrics. This evaluation includes metrics derived from the Productivity and Sustainability Improvement Planning (PSIP) and the Interoperable Design of Extreme-Scale Application Software (IDEAS) initiatives under the Exascale Computing Project (ECP). The presentation described the self-assessment process conducted for PSIP/IDEAS-ECP software, providing insights into productivity and sustainability enhancement planning within the context of future software development. Jai also showed progress in the TRANSP code modernization, Continuous Integration/Continuous Deployment (CI/CD), and Containerization. Additionally, he discussed the anticipated future needs for TRANSP software engineering, outlining key objectives aimed at significantly enhancing productivity, reliability, and portability. He also talked about possible improvements in TRANSP code infrastructure that are described in the next section.

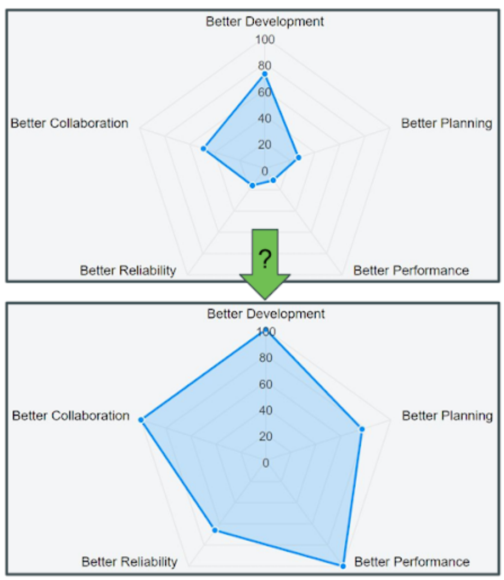

Figure 1: Towards the improvement of PSIP score in TRANSP (from J. Sachdev presentation [4])

2. Code Infrastructure, Core-Edge Coupling, and Engineering Integration

For future TRANSP code infrastructure, Jai Sachdev emphasized that the pursuit of a perfect PSIP score may not be necessary. Instead, it should be viewed as a guiding principle for continual improvement. The outlined strategic directions include a focus on achieving better reliability through the incorporation of unit testing and automatic deployment. Performance enhancements will be pursued through the addition of performance testing and the utilization of advanced portability libraries. Improved planning will involve a thorough requirements analysis, enhanced contribution management, and the establishment of guidelines. Additionally, development processes will benefit from integrated documentation within the release workflow.

The recent improvements made in these areas have not only facilitated the team's ability to address modernization tasks but have also minimized the risk of potential disruptions. There is still a clear path to improve the PSIP TRANSP score by improving TRANSP planning, development, collaboration, performance, and reliability as shown in Fig. 1.

Olivier Hoenen from ITER organization introduced concepts related to code coupling using the Integrated Modeling and Analysis Suite (IMAS), highlighting the numerous advantages associated with standardizing codes through IMAS Interface Data Structures (IDSs). The benefits include the ability to compare results and benchmark codes effectively, utilize machine-agnostic inputs, couple codes for trading physics fidelity for performance gains, and capitalize on community-developed toolboxes instead of reinventing solutions. Within IMAS, various tools are developed for different code-coupling patterns, providing support for initiating coupling processes or advancing to more complex levels. An essential milestone for IMAS is the move toward open sourcing. This shift toward open sourcing is envisioned as the foundation for a more dynamic and engaged community of contributors, all operating within a Fair, Accessible, Interoperable, and Reusable (FAIR) data environment.

Andrei Khodak presented the prospective applications of the TRANSP code within a virtual prototyping system for future tokamaks. Highlighting TRANSP's versatility, he talked about its capability to define crucial aspects within the virtual prototyping system, including plasma shape, neutron source distribution, and magnetic field configuration. Furthermore, Andrei discussed the potential for a two-way coupling system involving TRANSP and plasma edge codes. This envisioned coupling is important for several applications, such as for plasma-facing component development, prediction of heat and species flux profiles using coupled SOLPS-ITER/CFX simulations, and exploration of transient effects in liquid metal MHD studies. Andrei's presentation demonstrated the diverse and impactful potential applications of TRANSP within a virtual prototyping system, offering insights into the advancement of fusion research and device development.

The importance of core-edge coupling was also discussed in presentations by Brian Grierson from General Atomics and Michele Romanelli from Tokamak Energy. Grierson's insights provided a comprehensive perspective on extending TRANSP's applicability through core-edge coupling. He argued that there is a need to maintain a fundamental time-dependent solver while exploring opportunities to improve predictive simulations. Grierson's presentation underscored the importance of a unified analysis suite that seamlessly couples core and edge simulations, potentially transforming TRANSP into a more versatile tool.

3. Enhancing Interpretive Capabilities

A possible path towards improving interpretive capabilities was discussed in the presentation by Alexei Pankin. His proposal involves combining the existing comprehensive interpretive features within TRANSP with the creation of a novel interpretive modeling framework. This proposed framework integrates Bayesian methods and synthetic diagnostic tools with the TRANSP code. By doing so, it offers a robust platform for validating theory-based models and provides improved guidance for planning future experiments. This approach aims to enhance TRANSP's interpretive capabilities, facilitating more robust and versatile applications in fusion research.

Possible applications of Bayesian methods for data-efficient optimization in future research were discussed in the presentation by Aaro Järvinen from VTT Institute in Finland, who offered a systematic approach to quantifying uncertainty in the state of investigated systems based on available data. The primary focus was on leveraging Bayesian Inference (BI) algorithms to streamline the parameter calibration process when validating computationally intensive models for fusion plasmas. The significance of data efficiency in managing the computational demands of complex models was discussed, emphasizing the role of Bayesian optimization (BO) as a strategic solution. Aaro presented examples of Bayesian inference and Bayesian optimization projects closely linked to EUROfusion, showing the ongoing efforts to integrate these methodologies into fusion research practices. The presentation emphasized the transformative potential of Bayesian inference and optimization in expediting parameter calibration processes and enhancing the efficiency of computationally demanding models in fusion plasma research.

Paulo Abreu's contribution described the progress made in synthetic diagnostics and Heating & Current Drive (H&CD) workflow development within IMAS. This involves generating synthetic data, preparing for ITER data analysis using Bayesian modeling, and supporting controller development through the PCS Simu-

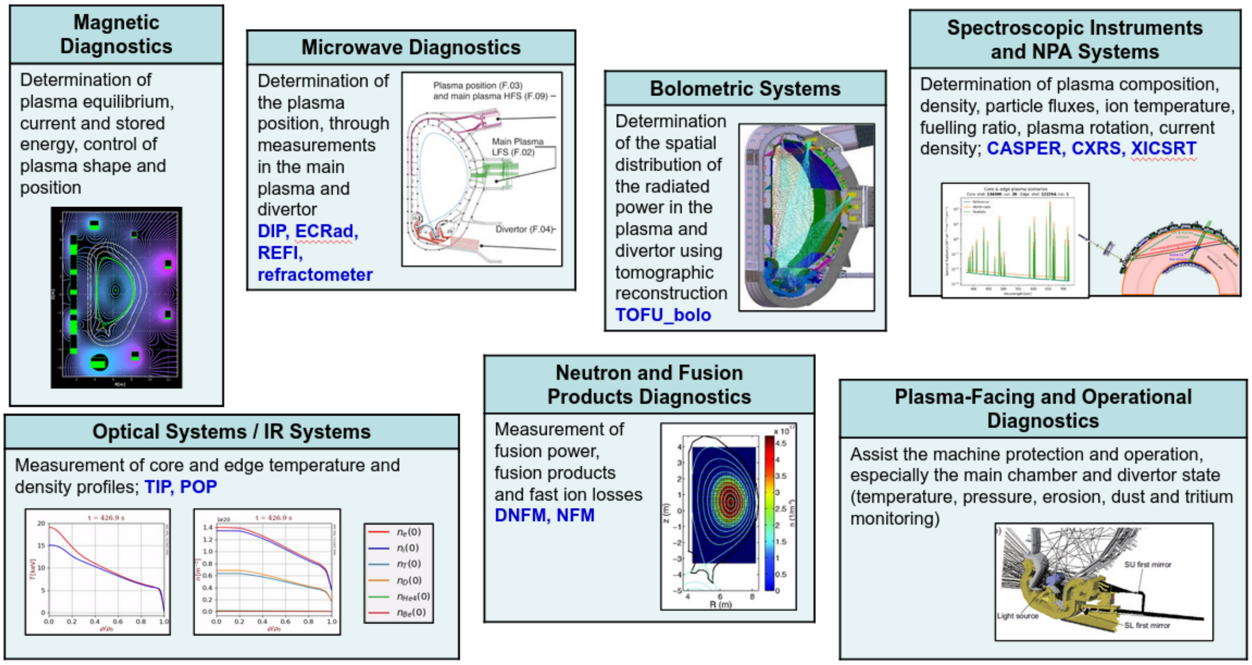

Figure 2: Examples of ITER synthetic diagnostic packages available through IMAS (from P. Abreu's presentation [5])

lation Platform. Additionally, IMAS facilitates the modeling of the synergy between various H&CD sources, particularly in connection with the High-Fidelity Plasma Simulator (HFPS). The presentation exposed ongoing preparations for additional workflows within IMAS, specifically tailored for ITER operation. These cover interpretive equilibrium reconstruction and stability assessments, including the evaluation of Edge Plasma (EP) effects. Overall, Paulo outlined the comprehensive and evolving role of IMAS in supporting various facets of ITER's research agenda, from high-fidelity simulations to data analysis and control system development.

Stan Kaye and Shaun Haskey from PPPL talked about needs for between-shot analysis for both NSTX-U and DIII-D operations. This type of analysis necessitates a close integration of TRANSP with data acquisition, storage, and equilibrium reconstruction to facilitate effective simulations between experimental shots. They emphasized the valuable insights that between-shot TRANSP runs can provide for control room decisions and preliminary assessments before going into more detailed studies. The utilization of TRANSP in this context enhances decision-making efficiency for session leaders, allowing for more informed and effective use of runtime resources. Stan and Shaun highlighted that much of the necessary infrastructure and scripts already exist, characterizing the challenges as predominantly related to system integration. According to Shaun, a substantial portion of research at DIII-D heavily relies on TRANSP analysis. From scenario development to transport and Edge Plasma research, TRANSP plays a foundational role. For any research related to plasma transport, an accurate power balance assessment is crucial—a task effectively fulfilled by TRANSP. The presentation emphasized the indispensability of TRANSP tools in evolving and monitoring the fast ion distribution function, current drive, torque, and interactions with Magnetohydrodynamics (MHD). These tools prove invaluable for interpreting EP and scenario development results. Shaun highlighted two key aspects: first, the use of TRANSP's fast ion pressure for reconstructing actual equilibria obtained, and second, the critical role of the fast ion distribution function in assessing edge plasma transport, without which diagnostic measurements would be of significantly reduced usage. In essence, Stan and Shaun's presentations conveyed that TRANSP is crucial for a diverse range of analyses at NSTX-U and DIII-D, providing vital data and tools for researchers to explore and comprehend different aspects of plasma behavior and transport phenomena.

4. Predictive Capabilities for Discharge Optimization

The current state of predictive capabilities in TRANSP was briefly described by Alexei Pankin. He talked about modularization efforts for PT_SOLVER, the module that is used for predictive modeling of plasma profiles for electron and ion temperature, electron density, and toroidal rotation profiles. He also shared the results of a recent comparison of predictive capabilities in the TRANSP and ASTRA codes by Joe Abbate. In his recent verification and validation studies, Joe compared predictions for electron and ion temperature profiles for a set of randomly selected DIII-D discharges computed with the TRANSP and ASTRA codes. In particular, he demonstrated that the results of TRANSP and ASTRA predictive solvers agree when the sources and equilibrium profiles are identical in TRANSP and ASTRA.

The presentations by Steve Jardin (PPPL), Jeff Candy (GA), and Bill Dorland (U. Maryland) compare the predictive solver algorithms in the TRANSP, TGYRO, and TRINITY codes. TGYRO focuses on finding steady-state solutions, whereas both TRANSP and TRINITY employ similar numerical techniques to determine time-dependent solutions for transport equations. Although TGYRO's numerical algorithm is faster, many physics scenarios need time-dependent solutions, as highlighted in various presentations, including Brian Grierson's. Despite sharing common numerical algorithms, TRANSP and TRINITY differ in their application due to TRANSP's utilization of reduced transport models, while there is a version of TRINITY that is specifically optimized for gyrokinetic models like the GX code. This distinction emphasizes the diverse approaches employed by these codes in addressing various physics problems and their unique strengths in predictive solver algorithms.

Nikolai Gorelenkov's presentation described the physics basis of integrating reduced and initial value simulations of Energetic Particles (EP) into the comprehensive device model of TRANSP, featuring examples with the RBQ and kick models. He presented instances of EP physics studies for both DIII-D and ITER. Nikolai addressed the challenges posed by Alfvén wave chirping and avalanches in spherical tokamaks (STs), particularly their role as primary mechanisms for fast ion losses in NSTX-U. Looking forward, the future development plans should involve the readiness of RBQ and NUBEAM to contribute to Strategic Initiative Working Groups, including ITER Research proposal preparation, Fusion Pilot Plant, and Core-Edge Integration. Ongoing and forthcoming efforts include optimizing NUBEAM for initial value simulations under realistic plasma conditions. This covers considerations for multiple physics factors such as ripple effects, plasma profiles, and Coulomb scattering. Additionally, Nikolai highlighted the importance of investigating microturbulence levels in future fusion devices and their effects on EP confinement, aligning with the International Tokamak Physics Activity (ITPA) initiative on EP/microturbulence interactions.

The importance of predictive modeling for tokamaks was outlined in several presentations, including talks by Jae-Min Kwon (KFE Korea), Brian Grierson (GA), Pablo Rodriguez-Fernandez (MIT), Michal Poradzinski (UKAEA), Michele Romanelli (Tokamak Energy UK), Jack Berkery, and Jon Menard (both PPPL).

Jae-Min Kwon's presentation highlighted the critical role of predictive simulations in fusion research, specifically through the use of the Digital Twin and KSTAR Virtual Tokamak Platform. Jae-Min emphasized the necessity for a platform at KSTAR that facilitates automated analysis of heating, transport, and the examination of transient events such as Vertical Displacement Events (VDE). This platform should also support plasma control studies. He highlighted the requirement for diverse transport and heating codes and proposed that predictive TRANSP could serve as an optimal platform for integrating these codes seamlessly.

Pablo Rodriguez-Fernandez's presentation centered on the imperative to enhance the robustness of predictive simulations within TRANSP. Additionally, he argued the need for additional verifications of the theory-based models for anomalous transport.

Michele Romanelli's presentation concentrated on addressing the needs specific to ST40. The primary emphasis was on enhancing predictive capabilities, particularly in terms of density predictions. The discussion also included key modules such as the pellet ablation module (core source), SOL model (edge source, divertor condition), and pedestal model tailored for STs.

The presentations by Brian Grierson, Jack Berkery, and Jon Menard were on the various needs related to ITER scenarios and FPP designs. Brian Grierson outlined three fundamental elements that are necessary for utilizing the TRANSP code in future fusion facility studies. These elements include:

- **Speedup:** Addressing the barrier posed by the time to solution, seeking ways to enhance computational efficiency.

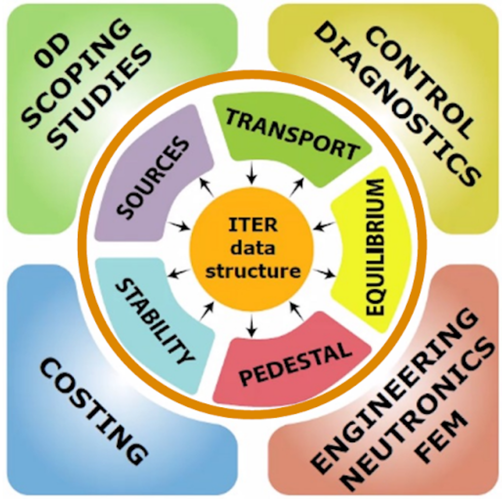

Figure 3: TRANSP provides a med+ fidelity plasma model at the heart of FPP design workflows (from B. Grierson's presentation)

- **Particle Transport Improvements:** (1) Introduce enhancements in particle transport to improve the realism for validation and predictions in burning plasma scenarios; (2) Incorporating theory-based impurity transport, isotope mixing, and refining fueling and pedestal density predictions.
- **Facility and Pulse Design Capabilities:** Incorporating user-defined features for coil layout, circuits, and passive structures to enable a more customizable approach to facility and pulse design.

These key elements emphasize the requirements necessary for utilizing the TRANSP code effectively in the context of future fusion facility studies, aiming for improved computational efficiency and enhanced predictive capabilities.

Jack Berkery presented critical improvements needed in the TRANSP code for more effective Fusion Power Plant (FPP) design studies. He also emphasized the need for clarity in choosing options for core thermal transport and advocated for the seamless integration of existing tools for edge integration within TRANSP. Additionally, he addressed concerns related to particle transport, specifically pellet fueling capability, and explored possibilities for providing output to external analyses. Overall, Berkery's presentation identified key areas of focus, ranging from improving specific functionalities to optimizing the integration of external tools to enhancing TRANSP's efficacy in the context of FPP design studies.

Jon Menard presented ideas for a TRANSP project related to recent changes in ITER's Plasma-Facing Components (PFCs) from beryllium (Be) to tungsten (W). The proposal involves utilizing TRANSP to recompute and update scenarios from the ITER Organization, assessing the impact of these changes on the US diagnostics and prioritizing the necessary modeling efforts accordingly. The plan includes implementing synthetic versions of the highest priority US diagnostics using IMAS and linking them to TRANSP. Further, TRANSP will be employed to model variations around reference scenarios, evaluating diagnostic sensitivity to scenario details. Jon Menard also suggested additional ideas for ITER, including the potential use of PPPL dropper technology for real-time boronization and the application of IMAS synthetic diagnostics for diagnostics implemented on WEST. This approach could serve as a platform for assessing impurity delivery and transport, with implications for ITER, KSTAR, and other facilities using droppers, contributing to an enhanced understanding of mass injection, edge impurity transport, and their impact on core confinement.

5. Summary and Discussion

The workshop featured a comprehensive exploration of various aspects related to the TRANSP code and its applications in fusion research. Researchers and experts presented insights into ongoing projects, future developments, and challenges associated with TRANSP. Key highlights included discussions on improving predictive and interpretive capabilities, leveraging Bayesian methods and synthetic diagnostic tools, and addressing the computational demands of complex models. Additionally, presentations touched upon the integration of TRANSP with IMAS, its potential applications in virtual prototyping for future tokamak systems, and its role in supporting ITER research plans. The workshop promoted the exchange of ideas, emphasizing the significance of TRANSP in advancing fusion science and technology. Participants also discussed specific needs for between-shot analysis, outlined improvements for Fusion Power Plant design studies, and proposed strategies for enhancing diagnostic sensitivity. The workshop provided a platform for researchers to share updates, discuss future directions, and collectively contribute to the development and optimization of the TRANSP code for diverse fusion-related studies.

The discussion that followed the presentations focused on the priorities of future TRANSP developments. Alexei Pankin emphasized the significance of TRANSP, citing its extensive user base and value in fusion research. He advocated for code flexibility, openness, and sharing specific components like PT_SOLVER and NUBEAM to attract external collaboration. The idea of positioning TRANSP as a potential candidate for the Fusion Design Center was discussed. A central task for this project could be the use of Bayesian methods and coupling with synthetic diagnostic tools to develop a new framework for theory model validation and verification. Marina Gorelenkova talked about the need to advance the physics basis while preserving user numbers, suggesting that IMAS could serve as a central focal point, particularly for ITER Diagnostic design. Pablo Rodriguez-Fernandez urged for increased transparency by making the TRANSP source code visible to users, emphasizing the benefits of modularization, possibly through IMAS. The strategic importance of continuing TRANSP was emphasized by Steve Cowley, contemplating whether to pursue a clean start or migrate the old version for continued interpretive analysis. Predictive TRANSP was highlighted as crucial components by several participants, aligning with the Fusion Predictive Center initiative. Jon Menard raised questions about TRANSP's competitive advantage and viability for advanced and spherical tokamak (AT/ST) fusion reactor plasmas, acknowledging its strength in this area while identifying weaknesses in pedestal, SOL, and divertor regions. He emphasized the need for a unified analysis suite with both predictive and interpretive capabilities. Bill Dorland addressed the challenge of incorporating high-performance computing capabilities into TRANSP to improve the fidelity of predictive modeling.

The discussion touched on the importance of interpretive analysis, the support required for synthetic diagnostics, the Virtual KDEMO project, and potential partnerships with facilities like KSTAR, TE, UKAEA, and SPARC. Nikolai Gorelenkov highlighted the global attention on the interaction between micro-turbulence and fast ions, advocating for new tools and recognizing the success of specific approaches.

The potential use of TRANSP in engineering analysis and design for fusion facilities emerged as an underexplored area, and the importance of addressing this gap was highlighted. The integration of engineering components into TRANSP aligns with Cowley's strategic considerations. This approach aims to position TRANSP not only as a tool for plasma physics but also as a comprehensive resource for engineering applications. The discussions touched upon potential rebranding and the transformative role TRANSP could play in AI-driven visual engineering.

The workshop discussion resulted in an agreement to investigate four key areas of development for the TRANSP code, with the intention of preparing whitepapers outlining research directions and required resources. The agreed-upon topics for further exploration are as follows:

- **Model Validation Platform:** There is an agreement to pursue the development of a model validation platform that integrates the TRANSP code with Bayesian methods and synthetic diagnostic packages. This initiative aims to create a robust platform for validating theory-based models, enhancing the interpretive capabilities of TRANSP, and guiding future experimental planning.

- **Improving Predictive Capabilities:** The workshop participants have collectively identified the need to enhance the predictive capabilities of TRANSP. The whitepaper for this area will outline strategies and resources required to advance TRANSP's predictive modeling, possibly incorporating gyro-kinetics to achieve high-fidelity predictions and surrogate models to achieve faster computations.

- **Extension to Edge Region:** The discussion highlighted the importance of extending the TRANSP code to the edge region. This involves coupling TRANSP with edge codes and utilizing it for both interpretive and predictive analyses in this critical area. The whitepaper will provide a roadmap for this extension, addressing challenges and outlining the necessary resources.

- **Coupling with Engineering Components:** Participants have expressed a shared interest in exploring the coupling of TRANSP with engineering components, which could lead to its use in a virtual prototyping system. The whitepaper will detail the prospective development and application of TRANSP in this context, specifying the resources required for successful integration.

By focusing on these four strategic areas, the TRANSP community aims to advance the capabilities of the code, addressing both current challenges and future opportunities in fusion research. The whitepapers will serve as comprehensive guides outlining the research directions, methodologies, and necessary resources for each of these initiatives, fostering a collaborative and informed approach to the future development of the TRANSP code.

In conclusion, the workshop discussion underlined the nature of the TRANSP code's future, bringing together user engagement, code transparency, predictive modeling, strategic planning, and collaboration with various fusion research initiatives and facilities. The challenge of finding the right balance between preserving TRANSP's strengths and addressing gaps was a recurring theme, emphasizing the need for a thoughtful and ambitious approach to secure its continued relevance in advancing fusion science and technology. The seamless integration of predictive and interpretive capabilities, core-edge coupling, and engineering components signifies a strategic vision for the future of TRANSP in fusion research.

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