PPPL PRINCETON PLASMA PHYSICS LABORATORY

PRINCETON UNIVERSITY

New Capabilities in the TRANSP Code

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Objectives of recent developments

Computation speed:

- NUBEAM optimization make its suitable for between shot analysis

Fidelity:

- TRANSP/T3D/GX simulation enabled, with embedded turbulence

Efficiency:

- IMAS conversion completed, providing uniform/standardize interface

Modularity:

- New TORBEAM and TORIC installed using IMAS interface

ML/AI Readiness:

- SI WG planning and ML/AI and BI provides a basis of TRANSP contribution to ASCR

FAIR4RS (Findable, Accessible, Interoperable and Reusable):

- We invite developers to contribute to TRANSP development

Outline of Activities

- **Optimization of NUBEAM on GPU**
- **T3D/GX interface in TRANSP**
- **Completion of the IMAS transition**
- **SI WG TRANSP activity**
- **TRANSP resources**

Mapping of Activities to Code Improvements

- Optimization of NUBEAM on GPU → Computation speed
- T3D/GX interface in TRANSP → Fidelity
- Completion of the IMAS transition → Efficiency, Modularity
- SI WG TRANSP activity → ML/AI Readiness
- TRANSP resources → FAIR4RS

Outline

- **Optimization of NUBEAM on GPU**
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NUBEAM optimization speeds by factor >20x. High resolution between-shot-analysis possible

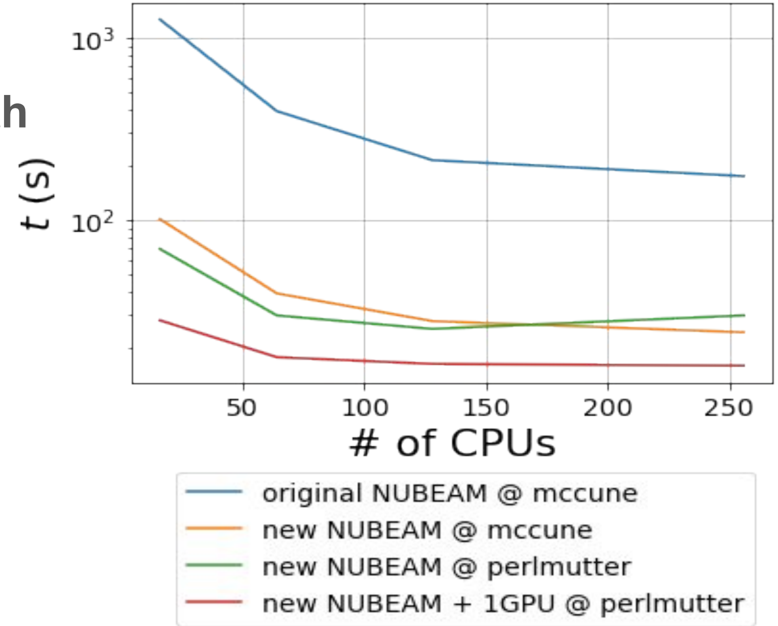
DIII-D Super-H mode discharge 174783 during high ion mode with dynamically changing parameters is selected

- Dynamic is followed in interpretive analysis with TRANSP-NUBEAM

With all optimization work done so far, NUBEAM simulation with 160k MC particles remains within 16 sec and is suitable for between-shot-analysis

- Code refactoring and modernization yields speedup of more than x 12
- Use of more modern computer architecture results in additional speedup of x 1.4
- Use of one GPU yields additional factor of x 2

Simulation for DIII-D discharge 174783 between 1.8 and 2s with 160k MC particles



Saturation in scaling is related to optimal # of MC per CPU and GPU

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T3D with GX brings embedded turbulence to TRANSP

TRANSP integrated code has

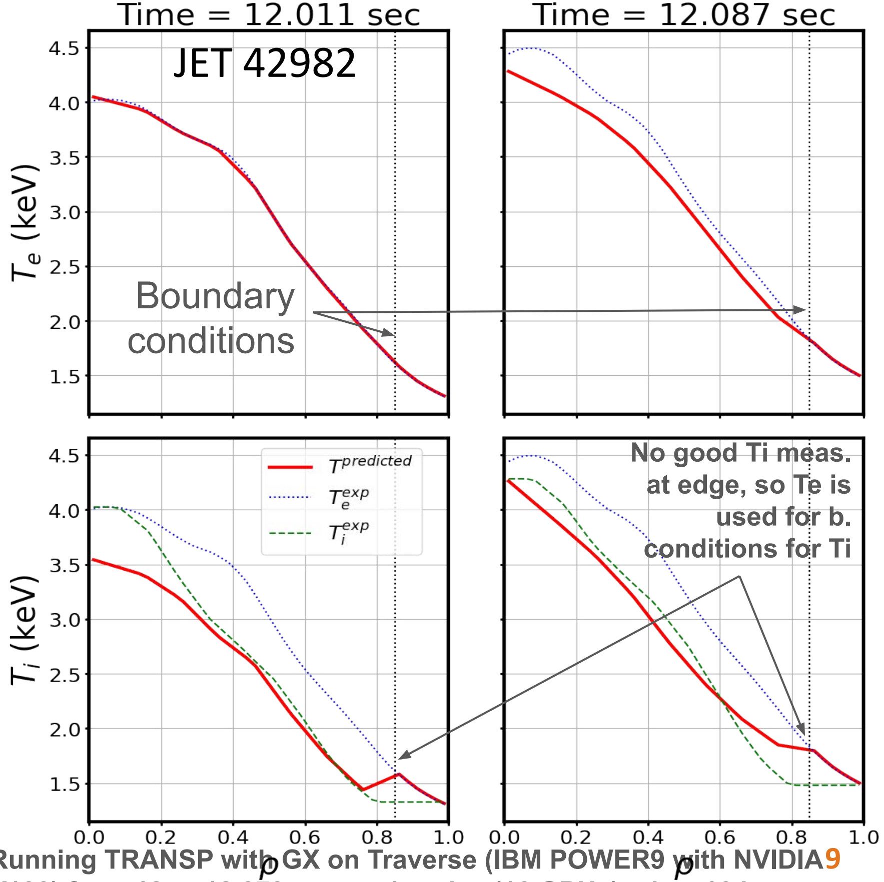
- **Large selection of sources for H&CD**
  - NUBEAM, TORIC, TORAY, TORBEAM, GENRAY, CQL3D
- **Free- and fixed boundary equilibrium solvers**
  - TEQ, ISOLVER
- **Models for large scale events (sawteeth)**
- **Pedestal models**
- **Synthetic diagnostics**
- **Selection of reduced anomalous and neoclassical models for plasma profile prediction**

PT_SOLVER is native predictive solver in TRANSP is developed as a modular solver, opening a path towards alternative solvers and models

Initial test with T3D/GX shows stability of coupling scheme

For the first time, high-fidelity gyro-kinetic GX model for anomalous transport [https://arxiv.org/abs/2209.06731] is implemented in TRANSP using the T3D/TRINITY transport solver

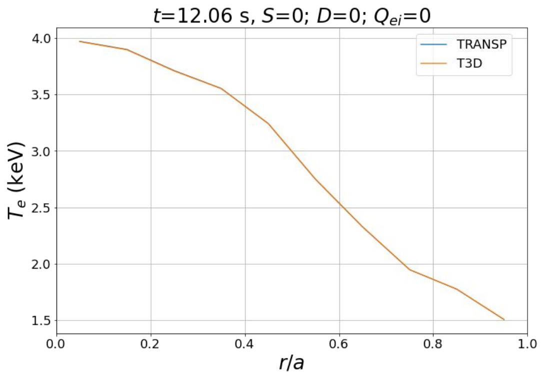
- **Solvers, equilibrium and plasma profiles are evolved self-consistently in coupled simulations**
  - TRANSP Ufiles and PlasmaStates are used for the code coupling
  - TRANSP uses multiple CPUs to compute sources and multiple GPUs for compute fluxes in GX

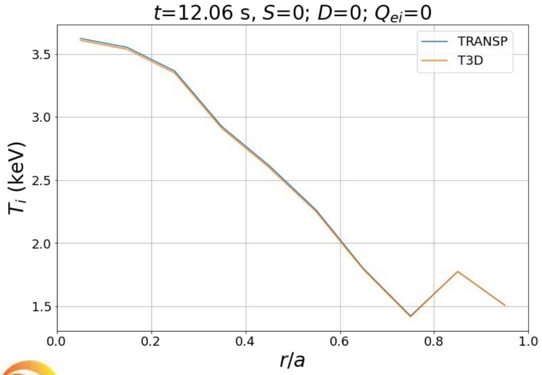


Running TRANSP with GX on Traverse (IBM POWER9 with NVIDIA V100) from 12 to 12.079 sec on 4 nodes (16 GPUs) takes 16 hours

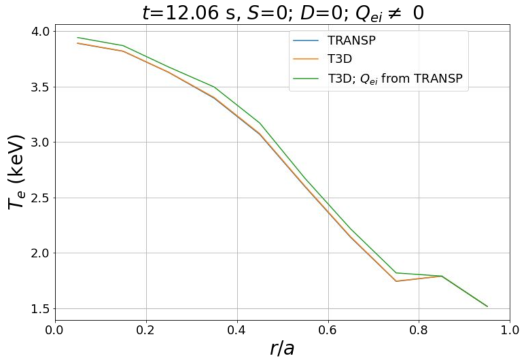
Successful verification of PT_SOLVER/T3D

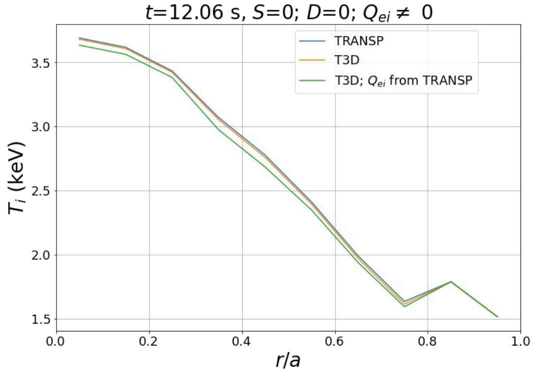
No sources/no transport/no Q_{ei}



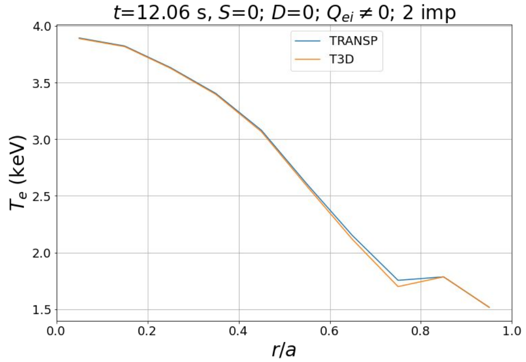


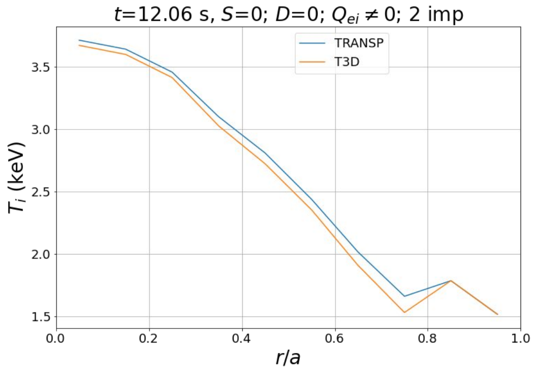
No sources/no transport/1 impurity/Q_{ei}





No sources/no transport/2 impurities/Q_{ei}





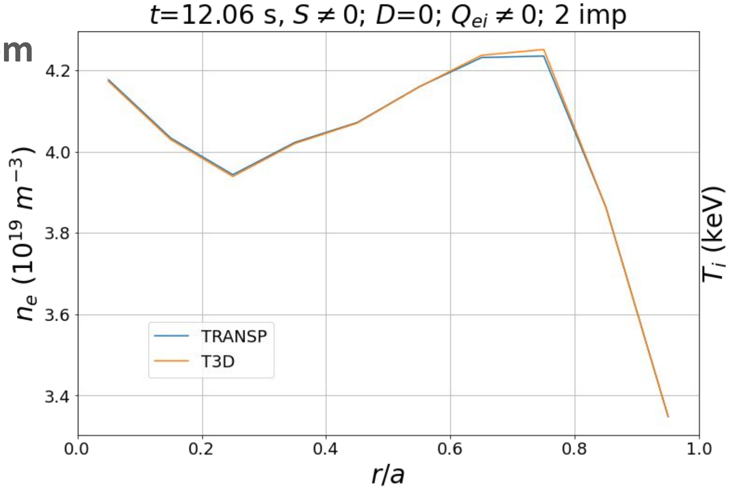
Successful verification of PT_SOLVER/T3D

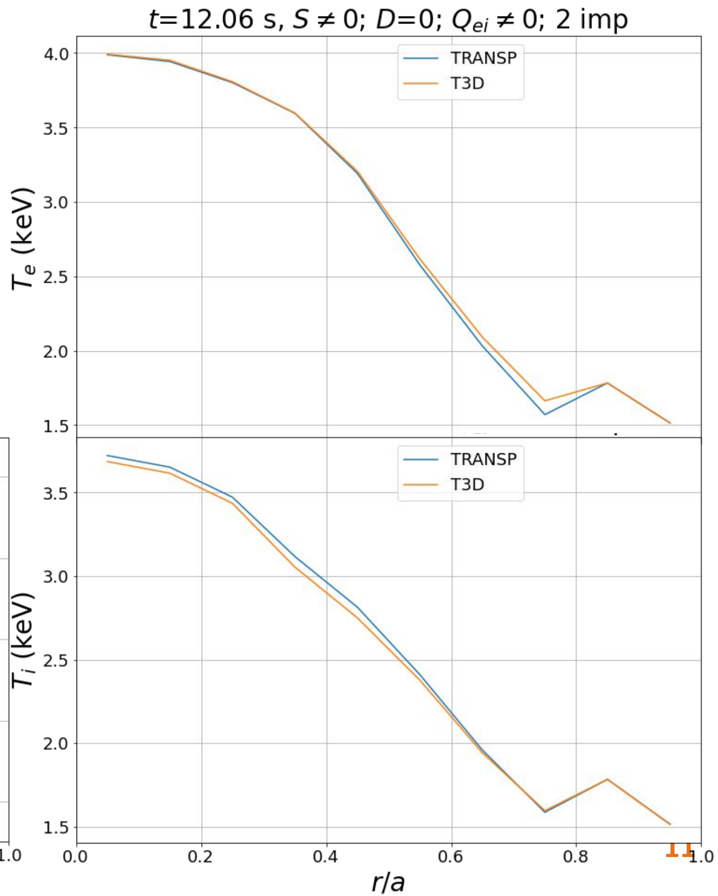
Separate T3D branch with TRANSP interface @bitbucket

- Reworked quasineutrality enforcement
- Supports multiple impurities

Small differences in predicted profiles

- In TRANSP, Q_{ei} is computed on a current time step after advancing density equation
- When T3D uses Q_{ei} from TRANSP, it is based on profiles from the previous time step
- There are other differences in Q_{ei} implementation in TRANSP and T3D

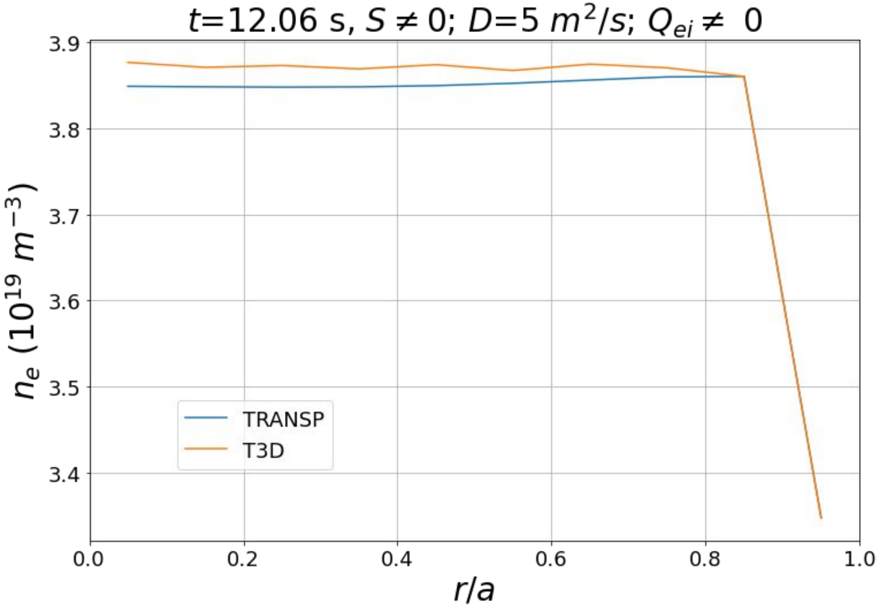




Verification of PT_SOLVER/T3D with transport shows small, but unexpected differences

USER model in TRANSP and RELU model in T3D can be compared if with RELU model stiffness set to 0

- Sources are computed in TRANSP (NUBEAM)
- Particular diffusivity is set to constant 5 m^2/s



After normalization, profiles are close, but they don't completely agree

… still work in progress

Current TRANSP/T3D/GX simulation can be used for interpretive stability analysis, but too slow for predictive analysis

- **GX is gyrokinetic code specifically developed for GPU platforms**
  - There are timescale separation in TRANSP for different processes in TRANSP
    - Time scales for equilibrium updates, source, and transport
    - Transport time scales are automatically updated based on how fast the profiles evolve
  - GX runtime depends on modes (instabilities) need to be resolved
    - Size of computation box/Run time to saturation
    - Individual computation for each time step is short: 0.035344 s / timestep in simulation that we try to resolve ITG modes in the JET discharge 42982
    - Total computation time of GX to saturated fluxes (normalized GX time=500) takes 256 minutes with transport time scale set by TRANSP of dt=0.001s
- **Still not ready for between-shot analysis**
  - Additional GPU improvements might be necessary
  - Potential hybrid models
- **However can be used for selected time slices for flux comparison/stability analysis in between-shot analysis studies**

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Why did we bring IMAS to TRANSP?

IMAS integration in TRANSP

- **IMAS is now the international standard for data sharing**
- **Boosts international collaboration**

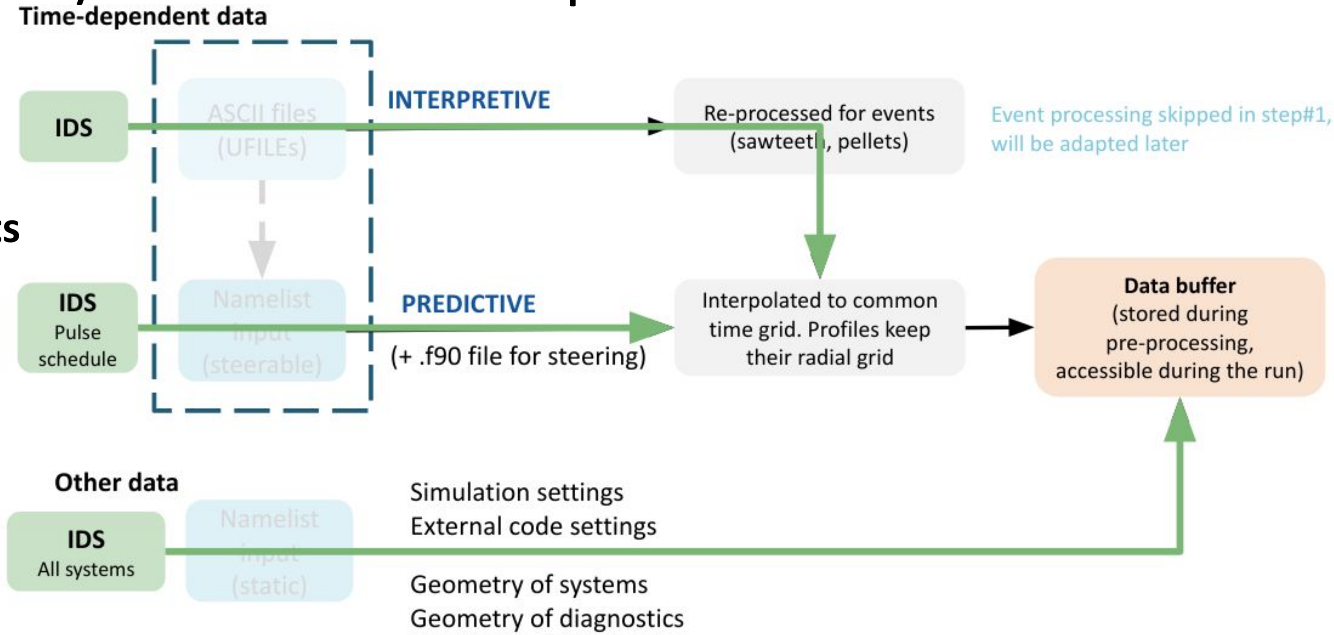
Advantages for US fusion program

- **IMAS integration strengthens US's position in global fusion program and accelerates adoption of best practices**
  - Access experimental data stored in IMAS (Europe, Asia)
  - Access ITER scenarios
  - Data can re-evaluated in TRANSP and stored in other convenient formats (such as MDSplus)

Funded by US Department of Energy (April, 2023 – June, 2024)

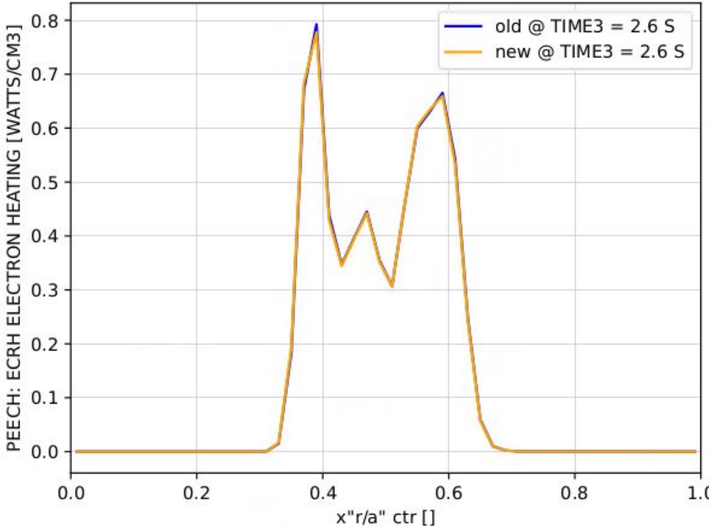
What has changed for users with IMAS?

- **IMAS interface develop in parallel with a legacy interface and remains optional**
  - **It is possible to compile TRANSP without IMAS**
- **IMAS provides new capabilities (data access, modules)**
  - **New python-based TRANSP/IMAS translator is developed**
  - **Currently able to run a TRANSP simulation (either predictive or interpretive) with inputs from IMAS database**
  - **New TORBEAM and TORIC models are implemented**



New TORBEAM and TORIC-6 implemented in TRANSP

- New version of TORBEAM
  - Implemented using IMAS interface and old interface for verification of generic EC/IMAS interface in TRANSP
  - Collaborated with TORBEAM developers on resolving name conflicts and proper deallocation of arrays inside TORBEAM



- TORIC-6 with IMAS interface; TORIC-5 is maintained using legacy interface
  - TORIC-5 and TORIC-6 are available in TRANSP for direct comparison
- New RF models are enabled using IMAS interface IC_MODEL/EC_MODEL = ‘IMAS’
  - RF model name specified rather specified in IMAS IDSs

New tool for free-boundary can be useful for FPP design studies

- **Free-boundary TRANSP Runs with ISOLVER:**
  - **Require precomputed Green's functions and mutual inductance matrices for coils and passive conductors**
- **Current Process:**
  - **Green's functions and matrices generated by *make_eqtok* during the library build stage**
  - **Relies on a pre-existing set of inputs for each device configuration, specifying:**
    - **Coil and conductor composition and geometry**
    - **Circuit connections and feedback systems**
    - **ISOLVER numerical parameters**
  - **Adding a new device/configuration:**
    - **Requires developer time and propagation to the next public TRANSP release**
- **New Approach *make_eqtok*:**
  - **Generates Green's functions and related data at runtime**
  - **Uses coil, circuit, and parameter information from IMAS (primarily *pf_active* IDS)**
  - **Offers faster turnaround and greater flexibility in configuration specification**
  - **Particularly useful for concept exploration**
  - **Still requires tuning and testing**

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SI WG TRANSP Follows TRANSP Workshop Recommendations

In addition to two technician tasks on optimization of NUBEAM for GPU and development of TRANSP/T3D interface, white papers are prepared on

1. **Model Validation Platform**
   Enhance model validation using Bayesian methods and synthetic diagnostics for better experiment planning
2. **Improving Predictive Capabilities**
   Integrate high-fidelity and surrogate models to boost predictive accuracy and enable faster scenario planning
3. **Extension to Edge Region**
   Expand core-edge coupling to provide detailed insights into edge plasma behavior and improve stability analysis
4. **Coupling with Engineering Components**
   Link TRANSP with engineering modules for virtual prototyping and advanced tokamak design studies

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4. **Coupling with Engineering Components**
   Link TRANSP with engineering modules for virtual prototyping and advanced tokamak design studies
5. **TRANSP for ASCR programs**
   Use its extensive databases and modeling capabilities to drive breakthroughs in fusion science and ML/AI, enabling innovative data-driven research

TRANSP for ASCR Programs

- ## ML/AI Model Development
  - **Would provide a platform for developing, employing, verifying, and validating ML/AI models, improving predictive capabilities and optimizing control strategies in fusion research**
    - **Examples of surrogate models used in TRANSP: EPED-NN, ELM triggering model for KSTAR**
- ## Bayesian Inference
  - **Would integrate Bayesian methods to enhance interpretive analysis, systematically incorporating prior knowledge and quantifying uncertainties**
- ## Data Management and Analysis
  - **Can facilitate the handling and analysis of large datasets from fusion experiments, contributing to improved data-driven discovery**
  - **TRANSP can be used to develop and test new methods for managing, curating, and analyzing vast amounts of scientific data generated by simulations and experiments**
    - **This aligns with ASCR's goals of improving data-driven discovery and enabling more efficient use of computational resources**
- ## Advanced Networking for Distributed Science
  - **Can support multi-institutional collaboration by leveraging high-speed networks for real-time data sharing and remote computation**
    - **Can contribute to the development of infrastructure that supports distributed science, a key objective of ASCR**

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We make code more open and welcome contributions following FAIR4RS: Findable, Accessible, Interoperable and Reusable

Please contact us if you want github TRANSP access. We will have updated license agreement to support this activity

Changes in TRANSP described in this talk are available in tshare TRANSP version released last week (TRANSP v24.4)

- T3D/GX capabilities are currently available only on perlmutter
  - Let's us know if you want to be a tester of these capabilities

Resources available for use

- TRANSP website: https://transp.pppl.gov
- TRANSP SIWG website: https://sites.google.com/pppl.gov/transp-siwg
- TRANSP paper: https://arxiv.org/abs/2406.07781
- Github repository for TRANSP support
  - To be included please send e-mail to transp_support@pppl.gov
- Contact us by email transp_support@pppl.gov
- Weekly TRANSP open office hours:
  - Every Monday at 11am ET
  - Zoom Meeting ID: 943 3131 5364
    Passcode: 82816439
- Monthly meeting with representative from ROs

Substantial TRANSP Upgrades over the past ~ 18 months to improve code capabilities and versatility

Thank you for your attendance - questions?

TORIC-6 is Implemented in TRANSP

- **TORIC-6 with IMAS interface is implemented in TRANSP; TORIC-5 is maintained using legacy interface**
  - Implemented with IMAS interface replacing old generic ICRH interface in TRANSP (uses core_profiles, equilibrium, ic_antennas IDSs)
  - Passing code-specific parameters through an XML string
  - Namespace conflicts resolved
  - Allow namelist specification of ICRF power when IDS is unavailable
  - Tested with ITER, DIII-D and ASDEX-U reference cases
- **Currently, both TORIC-5 and TORIC-6 are available in TRANSP for direct comparison**
  - Produce close results for reference case from DIII-D
  - However, there are cases when the models' predictions diverge
  - Opportunity, for direct model comparison within the same code

Implementation of TORBEAM and TORIC-6 use IMAS interface for Improved Modularity and Efficiency

- **It uses modular components for flexibility**
- **Standard interfaces for better integration**
- **New RF models are enabled using IMAS interface**
  IC_MODEL = 'IMAS'
  EC_MODEL = 'IMAS'
- **TRANSP input does not specify names of EC and IC models, but they are rather specified in IMAS IDSs**
- **Currently only one model for each EC and IC H&CD available**
- **This coupling scheme still requires TRANSP plug-ins for individual RF models**