Leveraging NERSC computing to support DIII-D operations through profile analysis and kinetic magnetic equilibrium reconstruction

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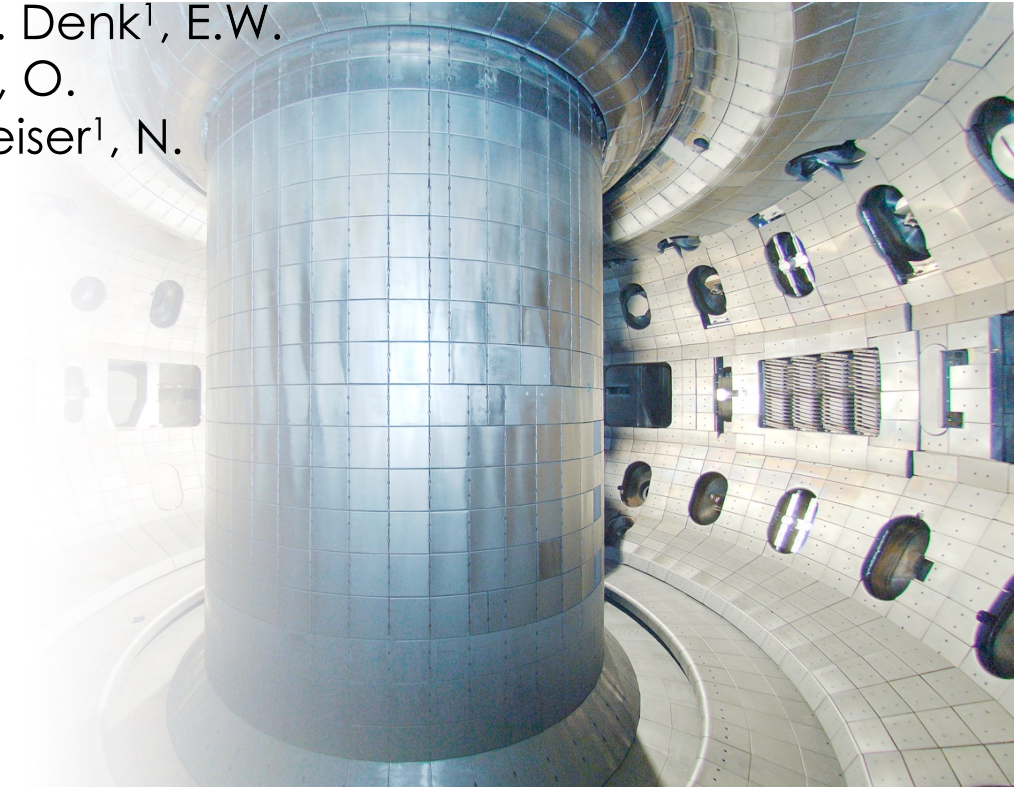


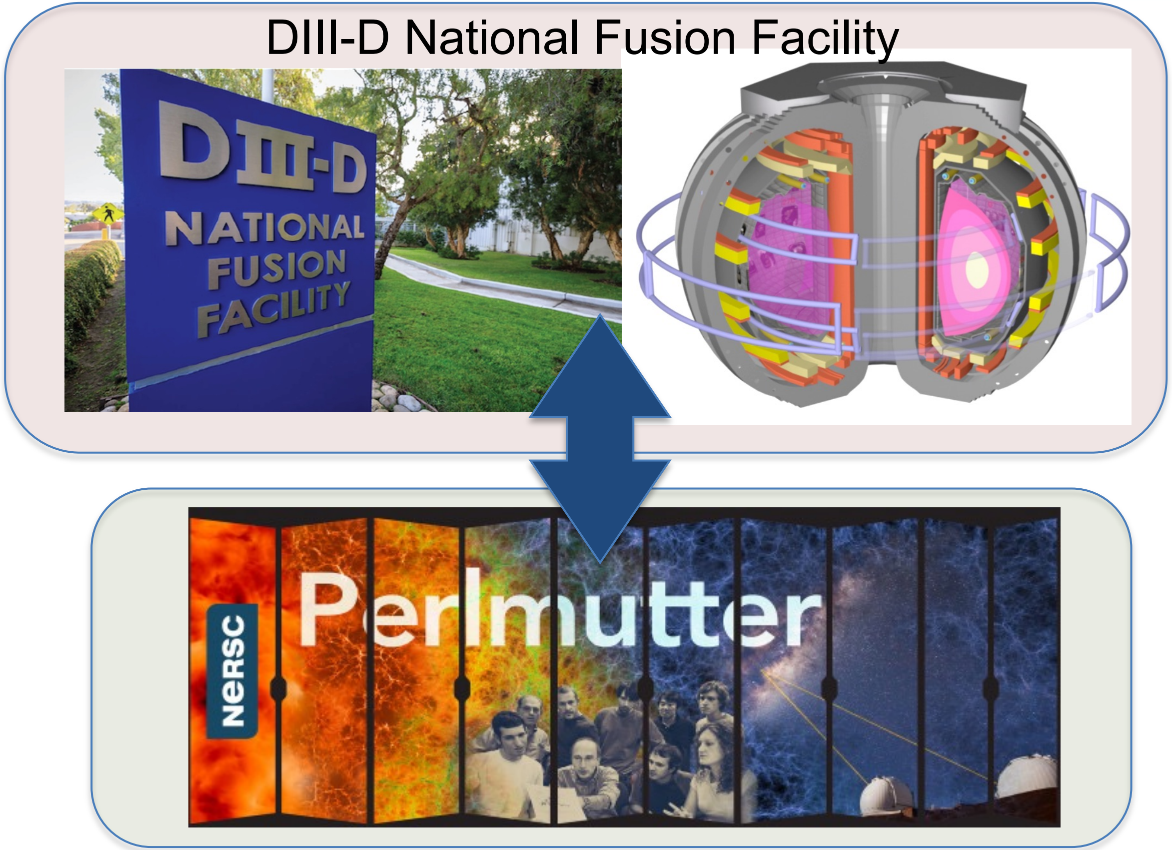
Presented at
The 4th Fusion HPC Workshop

Outline

- **Background and Context**
    - The super facility concept and history
    - Kinetic equilibria and the OMFIT/CAKE/EFIT workflow
- **Moving to NERSC computers**
    - Adjustments for broader applications
    - Profiling and optimization
    - Visualization and presentation
- **Result and performance**
    - Automatic processing of the previous D3D campaign
    - Comparison with manual kinetic equilibria
    - CAKE powered follow on analysis

NERSC D3D Superfacility established to provide timely analysis for decision making

- The ‘Superfacility’ concept aims to combine the experimental devices to cutting edge HPC facilities.
- Our project links the D3D National Fusion Facility to NERSC computing.
- It also seeks to demonstrate the feasibility of super facilities for future devices.

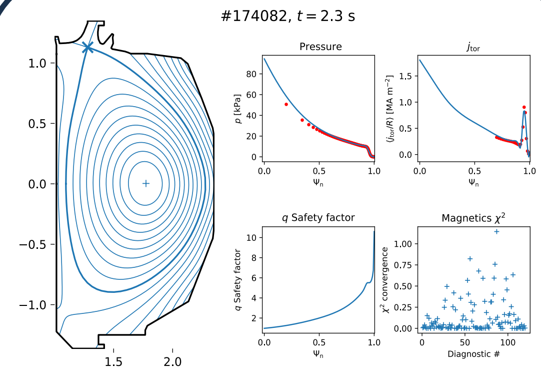


Experiences from previous HPC project implementing SURFMN provided valuable guidance

- Dedicated reservation at Argonne Leadership Computing Facility (ALCF)
  - March & April of 2017
- SURFMN analysis was run during relevant edge localized mode (ELM) experiments
  - 200 Plasma Shots
- Potential for between-shot coil decisions for ELM experiments
- Experimental scheduling was a concern. Computing needed to be pre-reserved.

[M. Kostuk, et al., 2018 Fus. Sci. and Tech., 74 135-143]

Kinetic equilibria is a foundational step to many fusion analysis workflows



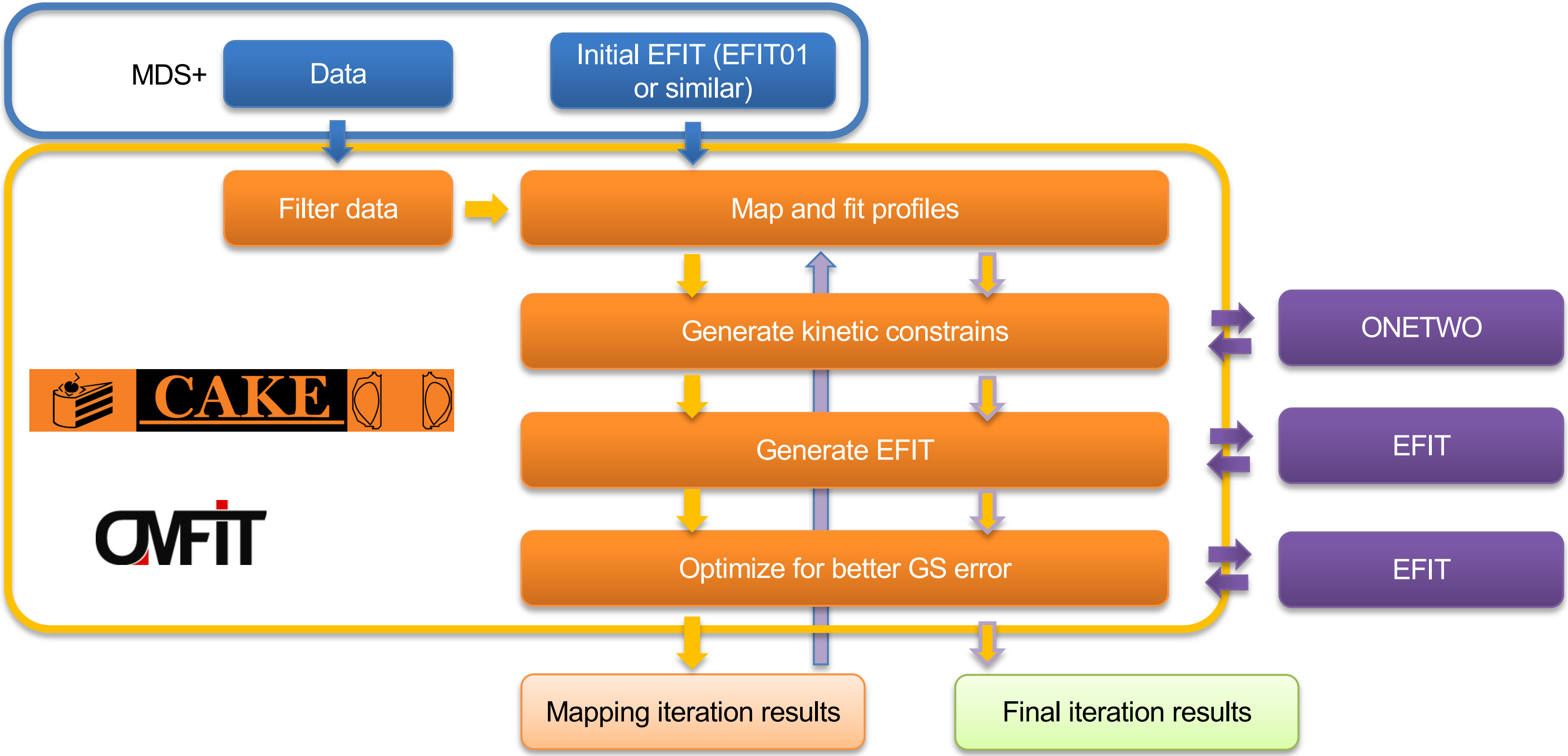
kinetic equilibria

MHD stability models (DCON, STRIDE, etc)

Transport models (TRANSP, UEDGE,etc)

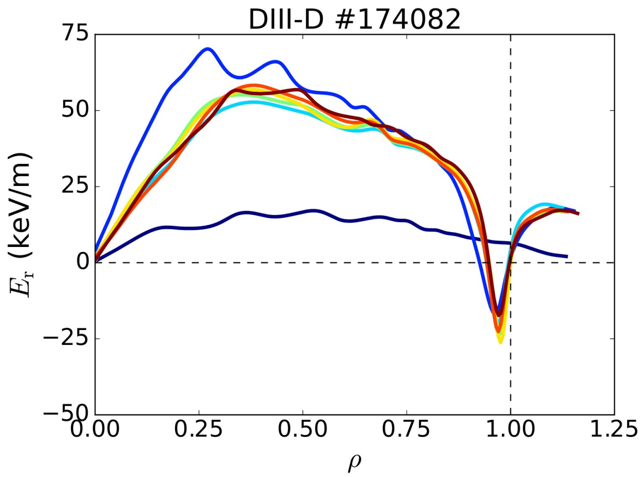
Gyrokinetic Simulations (TGLF, CGYRO, etc)

CAKE is a preexisting automatic kinetic EFIT workflow implemented in OMFIT

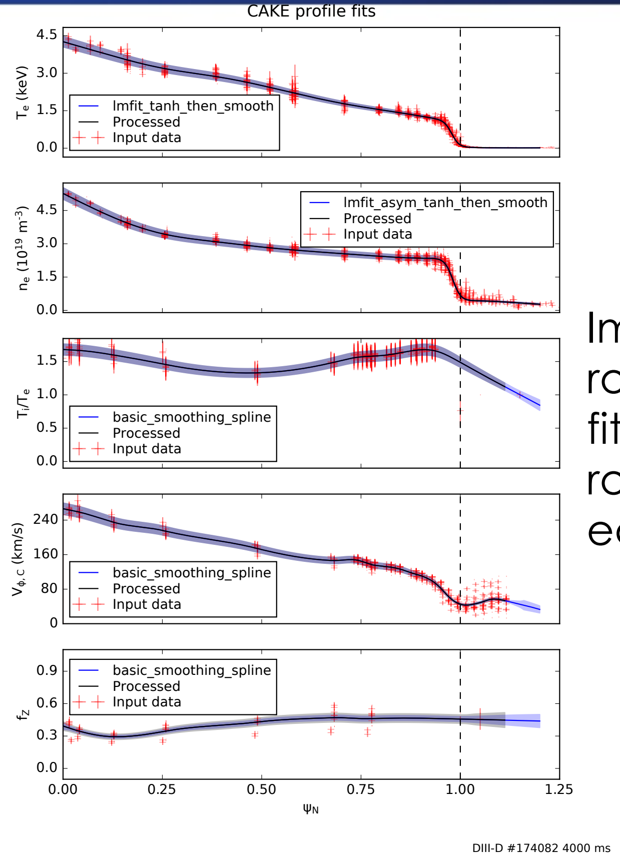


[CAKE workflow developed at Princeton University by Egemen group: Z.A. Xing, et al., Fus. Eng. Des (2021)]

Additional adjustments to CAKE made to suite a broader range of applications



Post fit Er calculations (colors represent different timeslices)



Improved rotation profile fitting for robustness and edge accuracy

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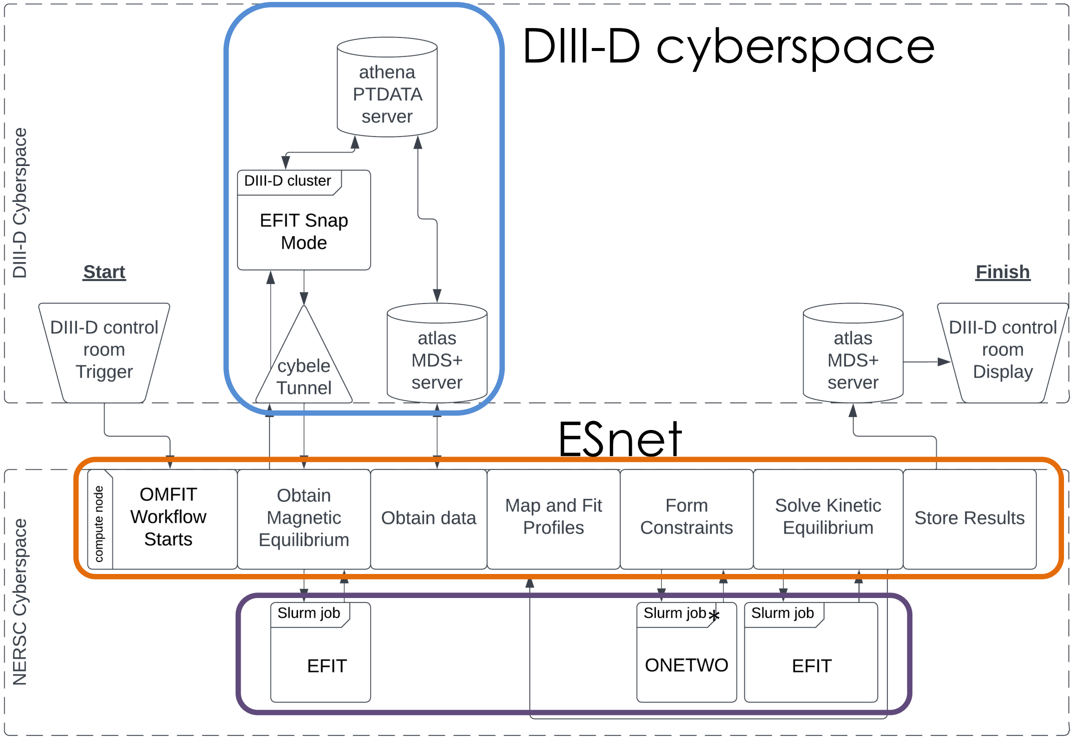
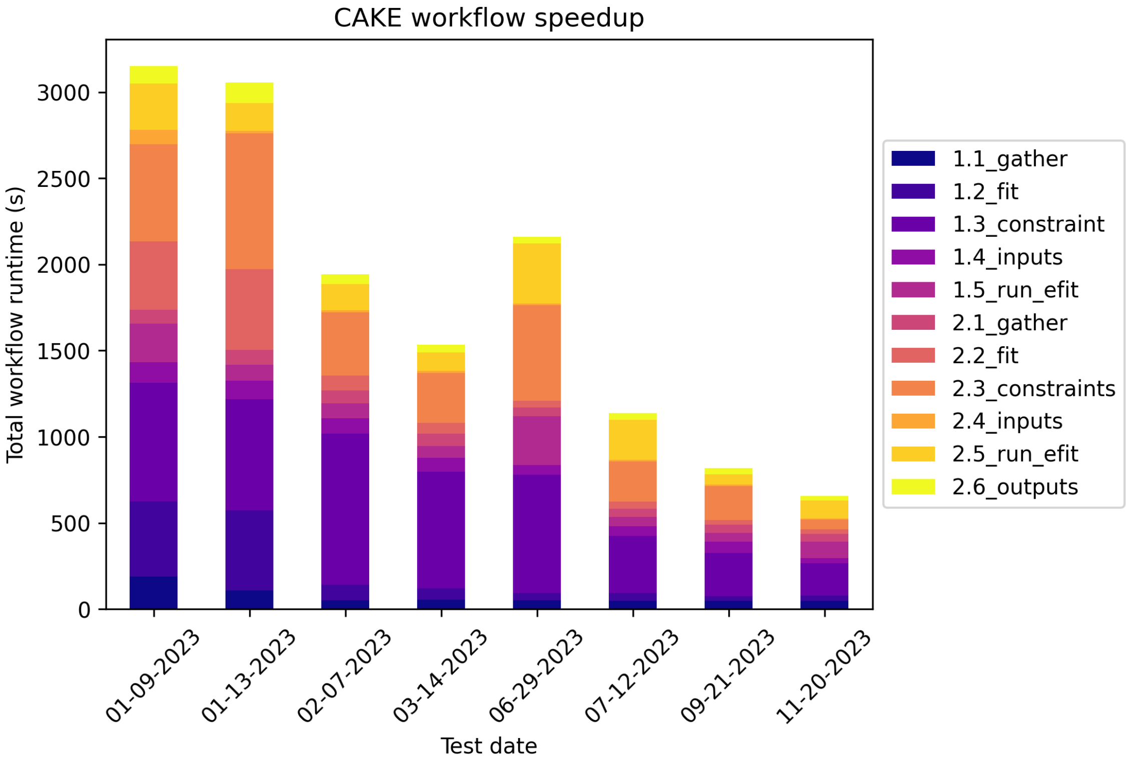
CAKE workflow has been adapted to NERSC computing with automatic triggering and data storage

- The D3D system automatically triggers the workflow when data is available.
- CAKE runs primarily on NERSC computers via the realtime queue.
- CAKE and OMFIT will fetch data from D3D's MDSplus database, as well run data packaging routines on D3D computers.
- The results are automatically uploaded to MDSplus upon completion.

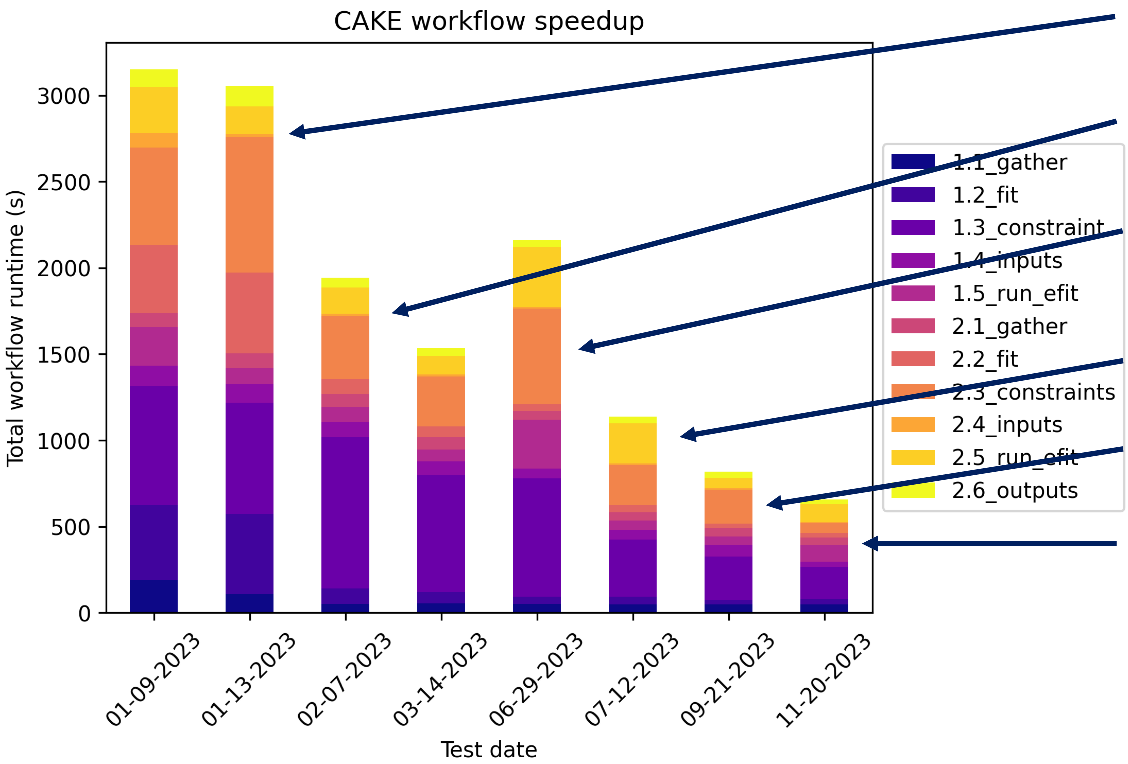


Workflow optimization and parallelization significantly shortened runtime



- Significant optimization work in areas of:
  - parallelization
  - streamlining of code logic
  - reduction in number of sophisticated objects created
  - decrease of slurm dependence
  - server dependent adjustments
- Benchmark runtime have decreased from ~ 53 min to 11 min.

Workflow optimization and parallelization significantly shortened runtime



Removed redundant data fetching and preparation

Initial parallelization effort

Moving to Perlmutter

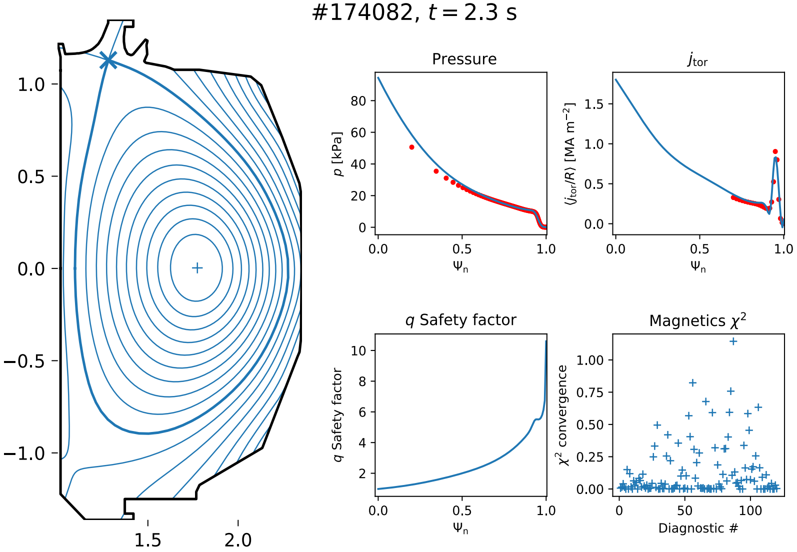
Perlmutter specific adjustments

Expansion of parallelization

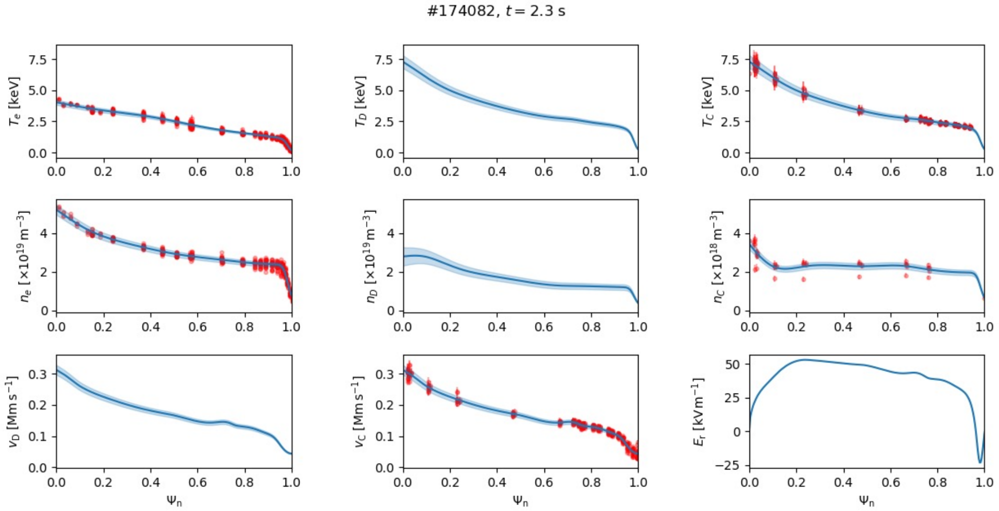
Reduction of slurm calls and parallelized file loading

Visualization tools developed to supplement existing tools

- Equilibrium reconstruction



- Fitted and calculated profiles



- Results can also be visualized using preexisting tools such as reviewplus and efitviewer

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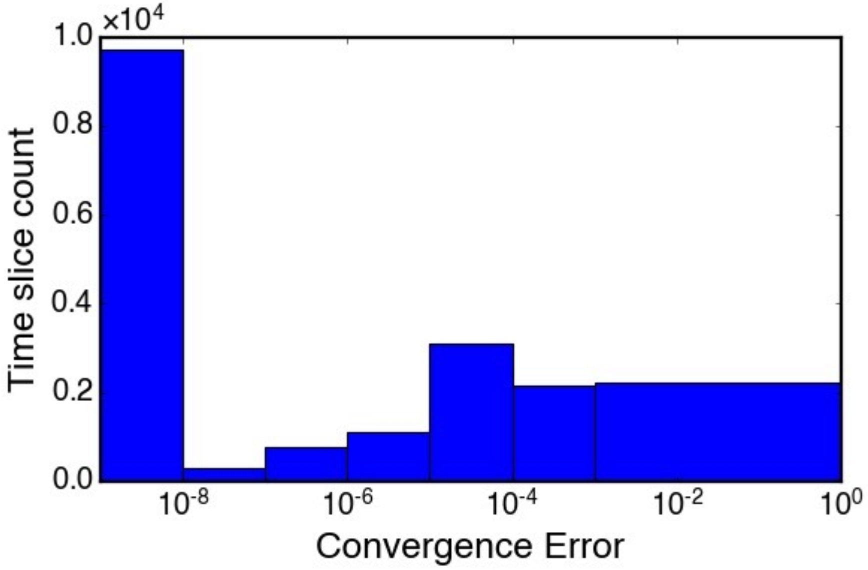
The CAKE workflow was run for the last D3D campaign

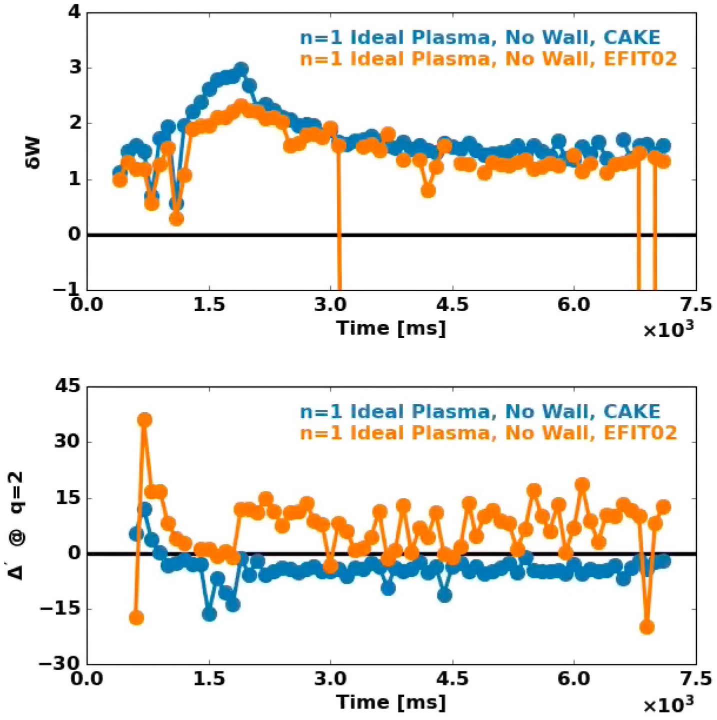
- During last D3D campaign 555 shots completed successfully
- 9742 of 19358 timeslices reached convergence error < 1e-8, typically required for stability analysis.
- Results are stored in MDSplus and can be used in follow-on workflows at NERSC or D3D.
- We anticipate being able to reach between shot timing for the upcoming campaign.



* 'classic' CAKE can achieve 90+% reaching 10-8 error, at the cost extra processing time

CAKE provides MHD stability insights not previously available

- When benchmarked against EFIT02 outputs in MHD stability calculations, CAKE results show:
  - global kink stability (δW) not changed significantly.
  - Local tearing drive (Δ') changes from destabilizing (Δ'>0) to stabilizing, reflecting actual plasma behavior.



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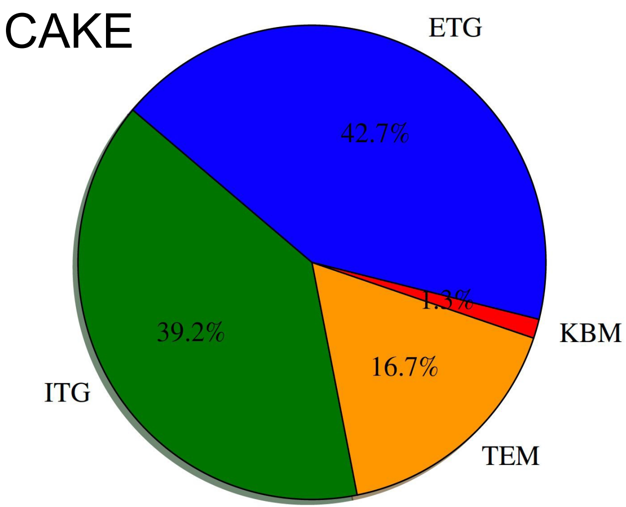
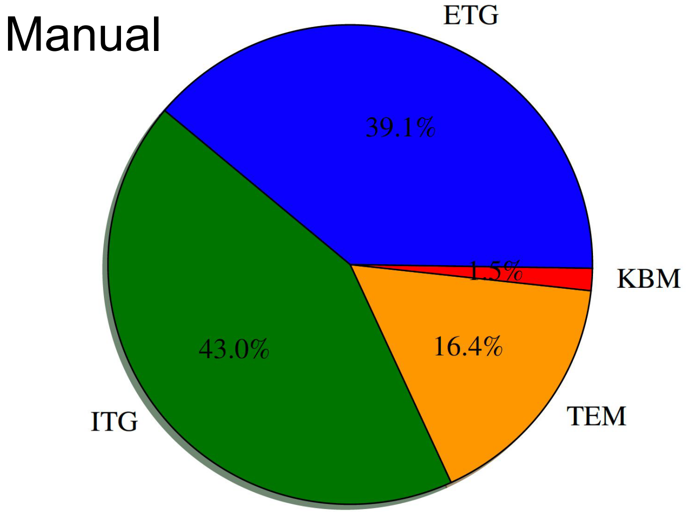
Database comparison between TGLF mode identification show similar model distribution

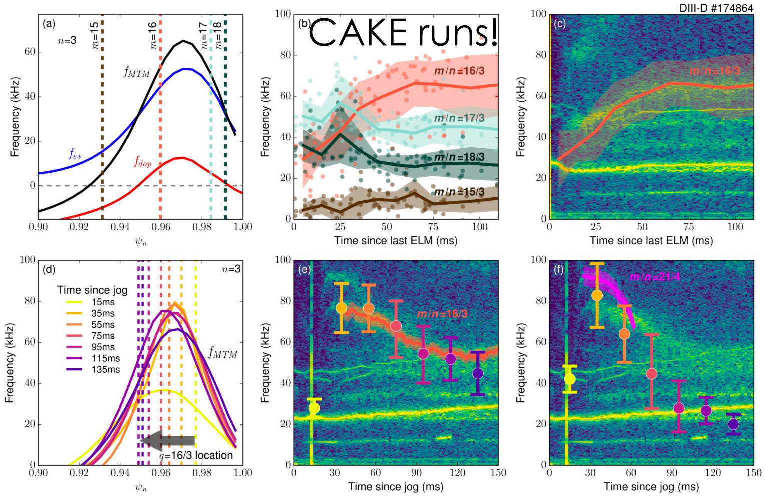
- A database of 1650 ‘manually’ made kinetic equilibria is used to compare to CAKE outputs for the same shot and times.





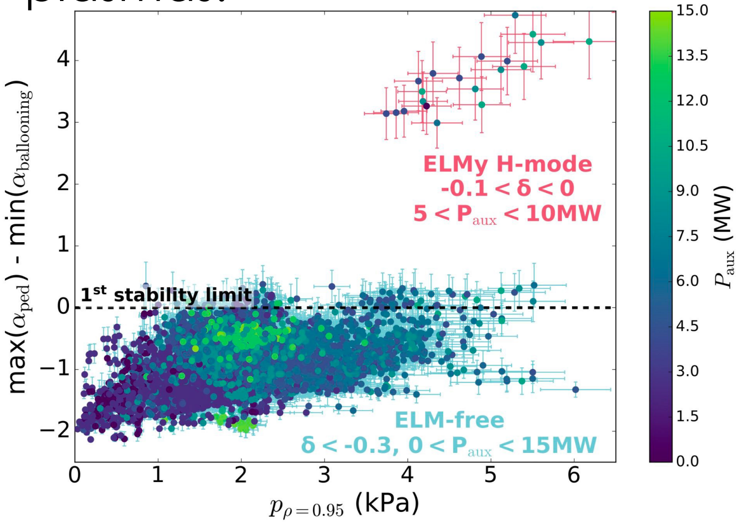
CAKE results have already contributed to important results and publications

- CAKE batch results showed preliminary MTM identification in plasma jogging experiment which was then confirmed and refined though manual analysis.



[Nelson et al. NF (2021)]

- BALOO modeling with CAKE results finds infinite-n ballooning stability prevents ELMS in negative triangularity (NT) plasmas.



[Nelson et al. PRL (2023)]

Future work

- Continue to streamline CAKE workflow
- Automate follow-on workflows
- Taking advantage of DOE Integrated Research Infrastructure initiative to diversify HPC centers where workflows can be run.
- Incorporation of other devices and workflows
- What would you want to accelerate?

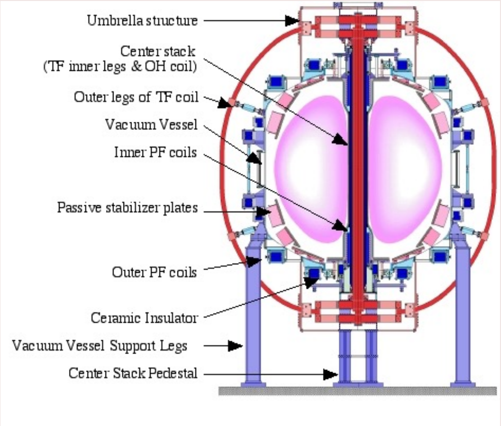
Acknowledgements

This material is based upon work supported by the US Department of Energy, Office of Science, Office of Fusion Energy Sciences, as well as the Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program under awards DE-FC02-04ER54698, DE-SC0022270, and DE-AC02-05CH11231.

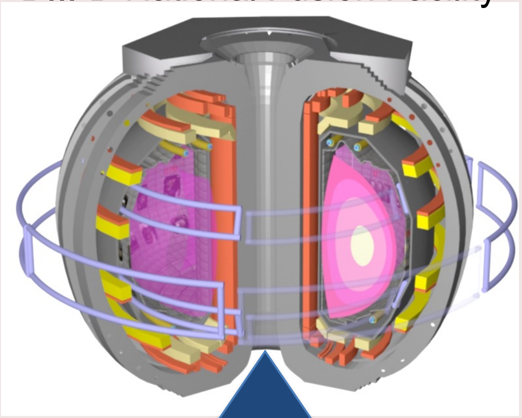
Extras! Extras!

Superfacility: Coupling ASCR High Performance Computing with other user facilities: Vision for Future

NSTX-U



DIII-D National Fusion Facility



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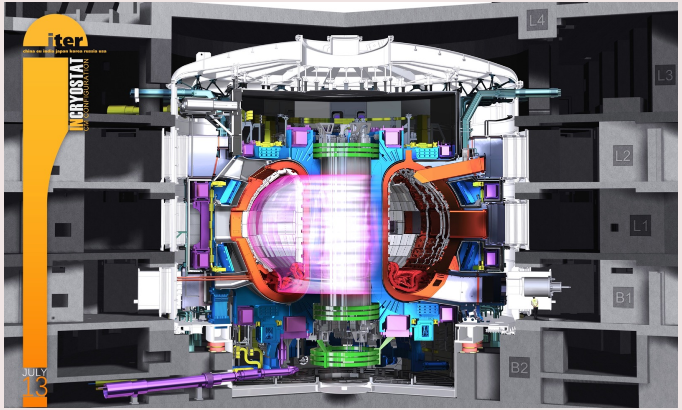

DIII-D NATIONAL FUSION FACILITY

Workflow profiling used to identify time sinks and bottlenecks

```
* * *  form_total_pressure_constraint.py 0.389s [N/A]
* * * *  record_err_flags.py 0.003s [0.0bytes]
* * *  calculate_currents.py 0.374s [0.0bytes]
* * * *  select_g_files.py 0.017s [0.0bytes]
* * * * *  check_outputs.py 0.009s [0.0bytes]
* * *  select_constraint_points.py 0.018s [0.0bytes]
* * *  check_current_constraint.py 0.031s [0.0bytes]
* * * *  select_g_files.py 0.004s [0.0bytes]
* *  4_MAKE_KFILES.py 7.542s [0.0bytes]
* * *  get_valid_times.py 0.002s [0.0bytes]
* * *  check_server.py 0.006s [0.0bytes]
* * *  choose_knots.py 4.061s [0.0bytes]
* * *  check_k_files.py 0.005s [0.0bytes]
* * *  tune_up_kfiles.py 1.807s [0.0bytes]
* * *  constrain_kfiles.py 1.527s [0.0bytes]
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* * *  manual_errors.py 0.047s [0.0bytes]
* * *  check_k_file_validity.py 0.044s [0.0bytes]
* * * *  record_err_flags.py 0.002s [0.0bytes]
* *  5_RUN_EFIT_WITH_KINETIC_CONSTRAINTS.py 88.773s [206.8MB]
* * *  check_server.py 0.006s [0.0bytes]
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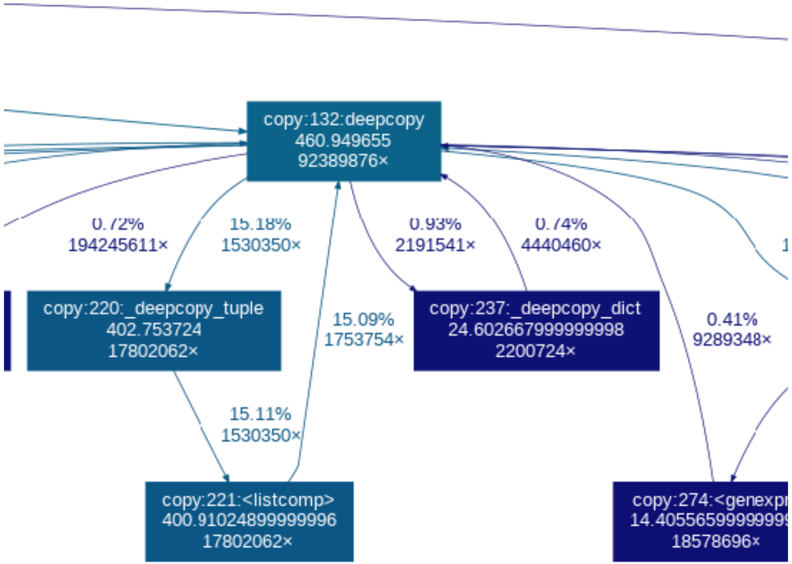

CAKE Workflow Segment	IRIS time	Perlmutter Initial	Perlmutter parallel run	Perlmutter qprint adjustment	Perlmutter 16 CPU	ONETWO adjustment and parallel loading
1_gather	154	53	51	50	49	50
2_fit	371	255	42	44	27	28
3_form_constraint (ONETWO)	675	789	697	331	250	190
4_make_k_files	130	76	55	55	66	28
5_run_efit_with_kinetic_constraint	380	348	286	55	52	96
2nd iteration						
1_gather	231	50	48	47	46	45
2_fit	362	223	40	41	27	27
3_form_constraint (ONETWO)	554	636	556	234	198	55
4_make_k_files	116	10	7	8	7	7
5_run_efit_with_kinetic_constraint	640	193	350	222	62	103
6_make_outputs	106	73	39	38	35	28
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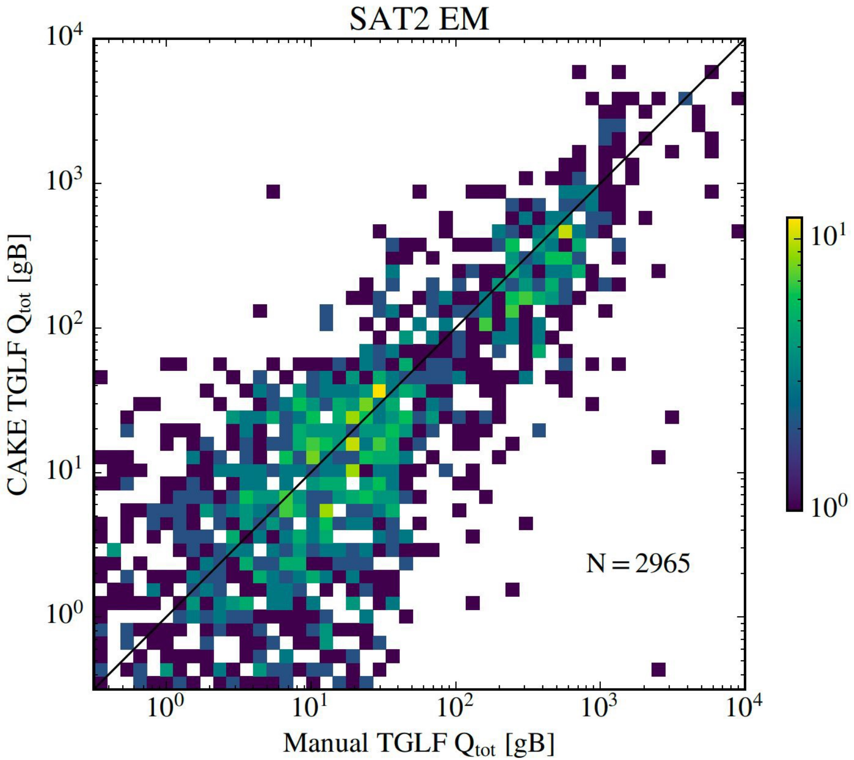
Total	3732	2713	2178	1131	823	662

* Includes variations on EFIT knot locations to get all slices below 1e-8 convergence error

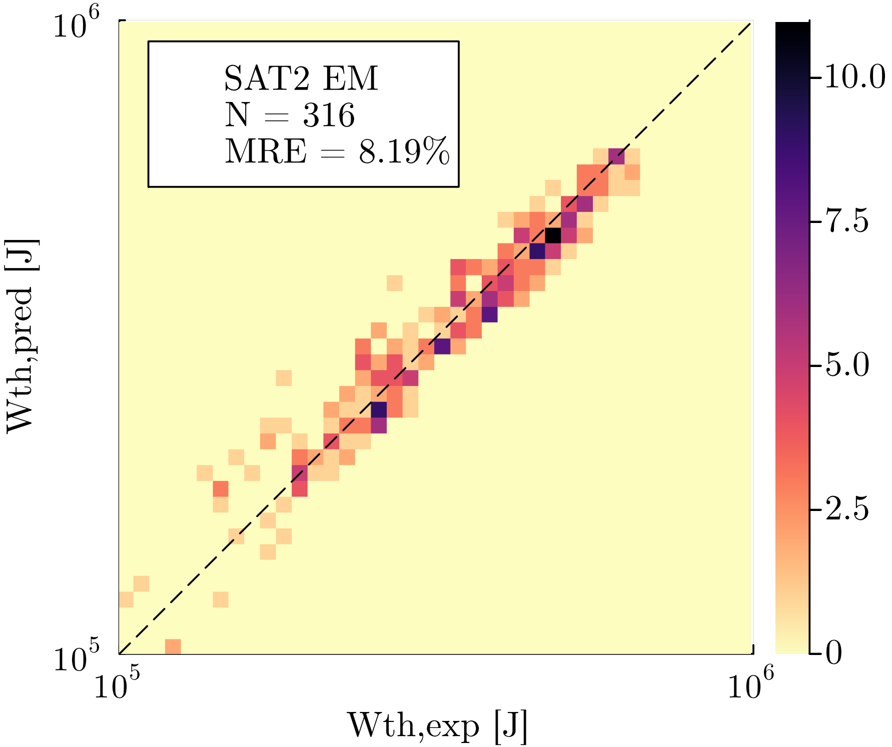
Comparison between TGLF results from based on CAKE vs manual equilibria show reasonable scatter

- TGLF ran using nominal profiles at ρ = [0.1, 0.2, … , 0.9]
- Heat flux comparison shows reasonable scatter comparable to experimental uncertainty
- However, scatter demonstrates well-known sensitivity of turbulent heat fluxes to profile information



CAKE results used in flux matched TGYRO simulations show great results in model prediction

- CAKE results (including ONETWO run) allow routine profile prediction with TGYRO flux-matcher (using TGLF-NN and NEO)
- Linear CGYRO(-NN) can be run on flux-matched profiles for identification of most unstable mode



Abstract

The OMFIT CAKE (Consistent Automatic Kinetic Equilibrium) workflow has been adapted and ported to NERSC's Perlmutter and Cori Supercomputers to provide profile analysis and kinetic magnetic equilibrium reconstruction for DIII-D control room use. The workflow has previously been implemented on DIII-D local clusters, but took long enough to be restricted to post experiment analysis. The new NERSC implementation uses between shot automatic triggering via the NERSC Superfacility API, runs on Perlmutter’s realtime queue, and connects with DIII-D via ESnet for timely data retrieval and writing of results to DIII-D’s MDSplus database. The workflow run time is reduced to 20 minutes by optimizations taking advantage of the greater opportunities for parallelization. Further improvements to usability include the addition of OMAS (Ordered Multidimensional Array Structure) based control room data visualization tools, improvements to profile fitting, and additional analysis. Work is continuing to integrate more advanced analysis post equilibrium reconstruction, including linking to TGLF and CGYRO gyrokinetic analysis as well as speed improvements to the internal high convergence workflow of the equilibrium reconstruction in order to accelerate production of low numerical error equilibria for MHD stability analysis.