Integrated Modeling of Core Tokamak Plasmas Accelerated with Surrogate Modeling and Uncertainty Quantification

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ABSTRACT

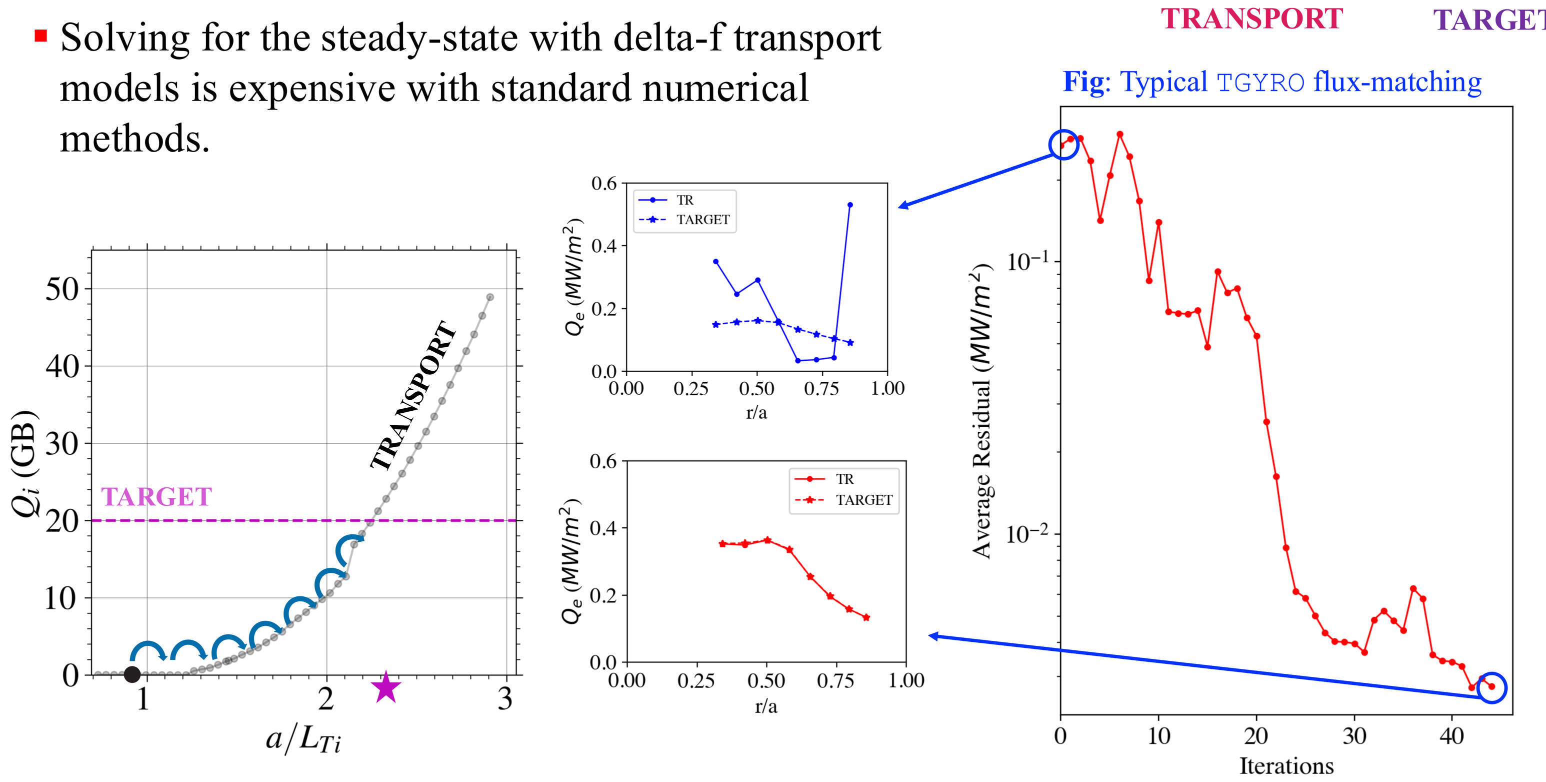
- Core integrated modeling of tokamaks involves the **multi-scale coupling** of core transport solvers for kinetic profile predictions, pedestal models, heating and current drive and MHD equilibrium codes, among other important physics aspects. Transport solvers with quasilinear turbulence models are often the **bottleneck** for the integrated simulations, representing most of the computational cost of self-consistent steady-state plasma predictions, particularly for burning and reactor-relevant plasmas.
- This work implements the **PORTALS** surrogate-based transport solver [1] into an **integrated modeling workflow** that loops over "black-box-type" simulation codes that solve for pedestal (using a surrogate to EPED [2] peeling-ballooning limits), Grad-Shafranov equilibrium, ion-cyclotron range-of-frequencies heating and Monte-Carlo alpha deposition. The latter physics aspects are resolved using interpretive TRANSP [3].
- This work demonstrates that this framework, named **MAESTRO** (Modular and Accelerated Engine for Simulation of Transport and Reactor Optimization), can provide **self-consistent steady-state solutions** of tokamak reactor cores with the full TGLF [4] reduced model for turbulent transport in a few dozen CPU hours and with minimal user input. The improvements to the PORTALS solver, performed under the **SMARTS SciDAC** partnership, are shown to provide an efficient, robust way to achieve steady-state solutions leveraging uncertainty quantification and physics-guided optimization methods.

1. PORTALS: FLUX-MATCHING AS SURROGATE-BASED OPTIMIZATION

- Kinetic profiles (and hence fusion performance) can be predicted solving steady-state transport equations:

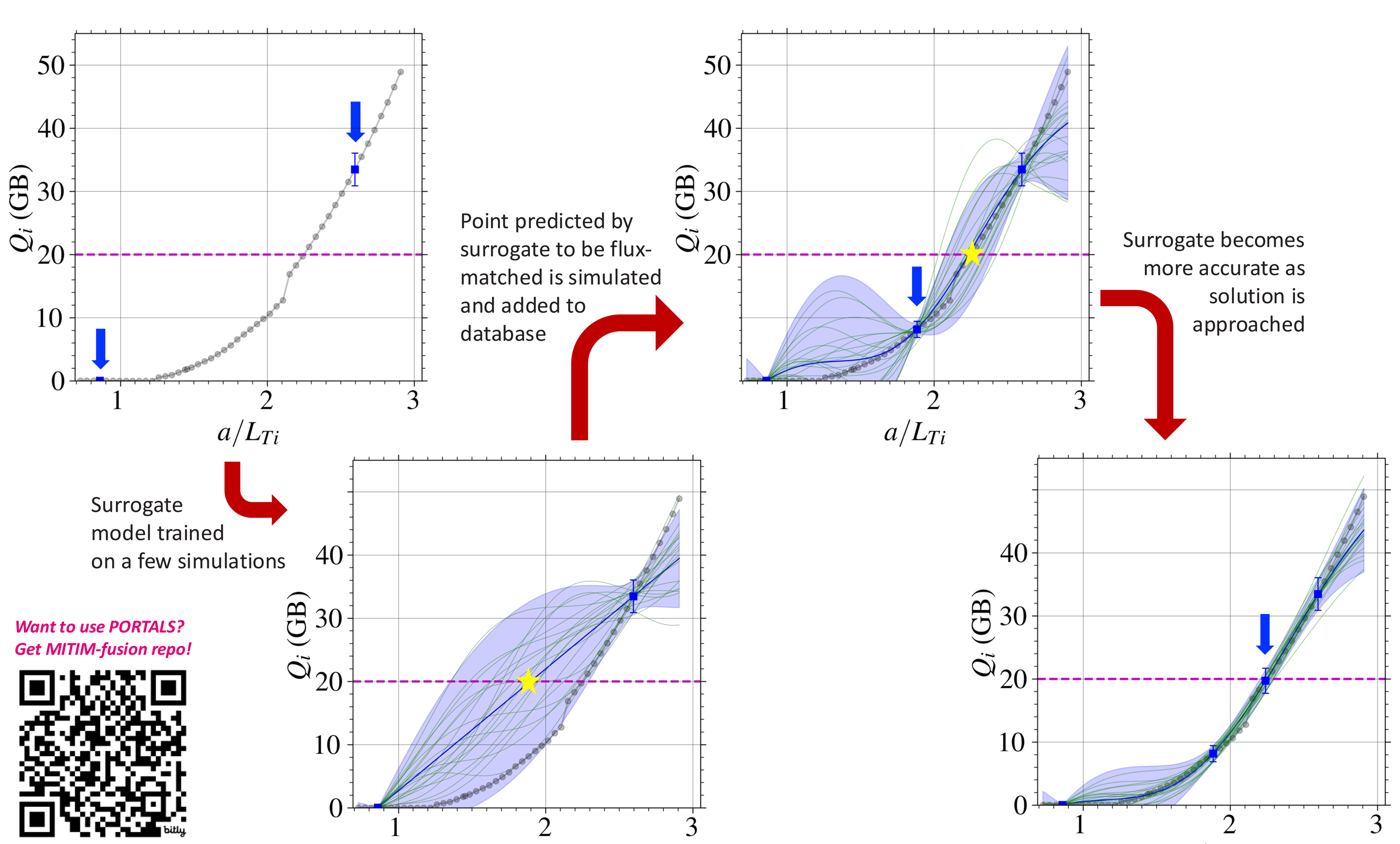
$$\frac{1}{V'}\left[\frac{\partial}{\partial t}\left(\frac{3}{2}n_iT_iV'\right)+n_iT_i\frac{\partial V'}{\partial t}\right]=-\frac{1}{V'}\frac{\partial}{\partial r}\left(\langle q_i\cdot\nabla r\rangle V'\right)+\langle S_i\rangle \Rightarrow \underbrace{\langle q_i\cdot\nabla r\rangle}_{\text{TRANSPORT}}=\underbrace{\frac{1}{V'}\int_0^r\langle S_i\rangle V'dr}_{\text{TARGET}}$$

- Solving for the steady-state with delta-f transport models is expensive with standard numerical methods.



- PORTALS [1] leverages surrogate-based optimization, suitable for expensive black-box functions.

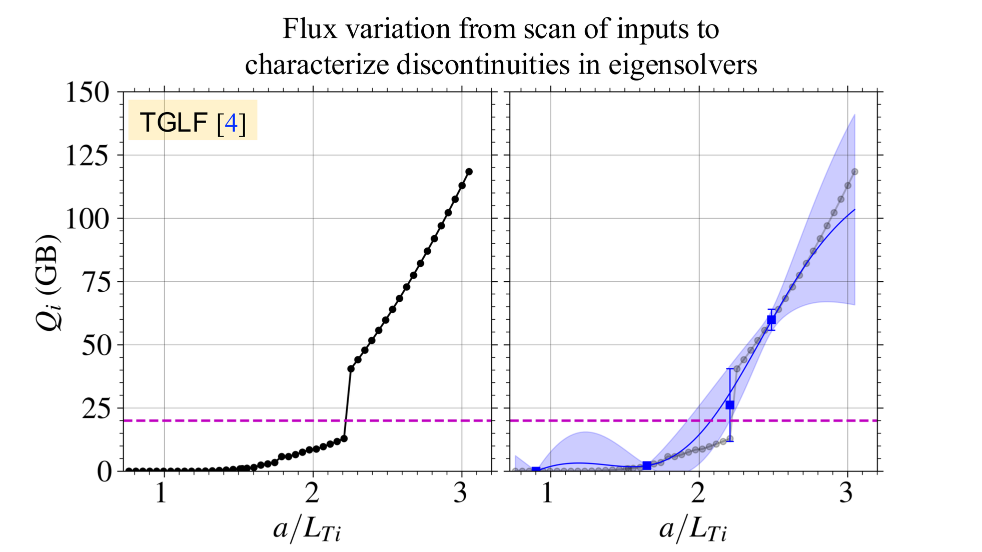
$$\underbrace{\langle q_i\cdot\nabla r\rangle}_{\text{TRANSPORT}}=\underbrace{\frac{1}{V'}\int_0^r\langle S_i\rangle V'dr}_{\text{TARGET}} \Rightarrow a/L_X^*=\text{argmin}\left|Q_i^{TRANSPORT}-Q_i^{TARGET}\right|$$

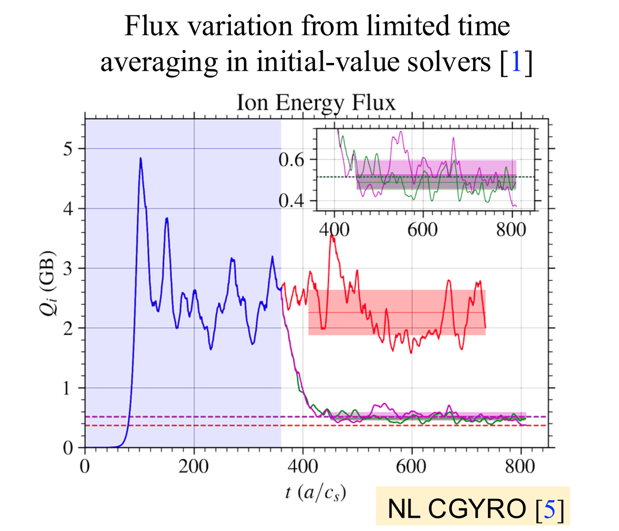


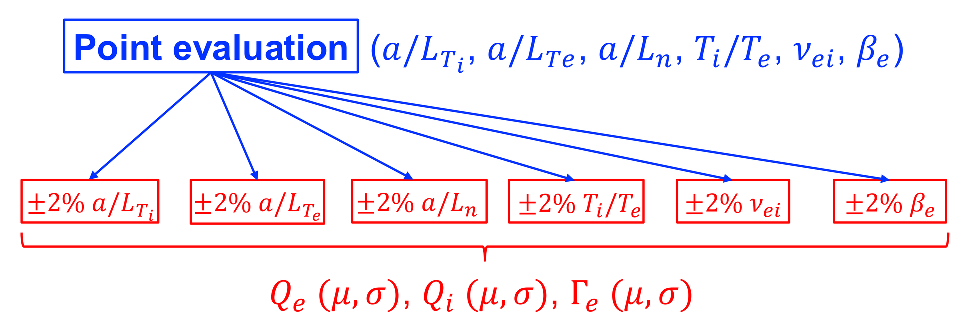
Want to use PORTALS? Get MITIM-fusion repo!

2. DEVELOPMENTS FOR ROBUST QUASILINEAR PREDICTIONS

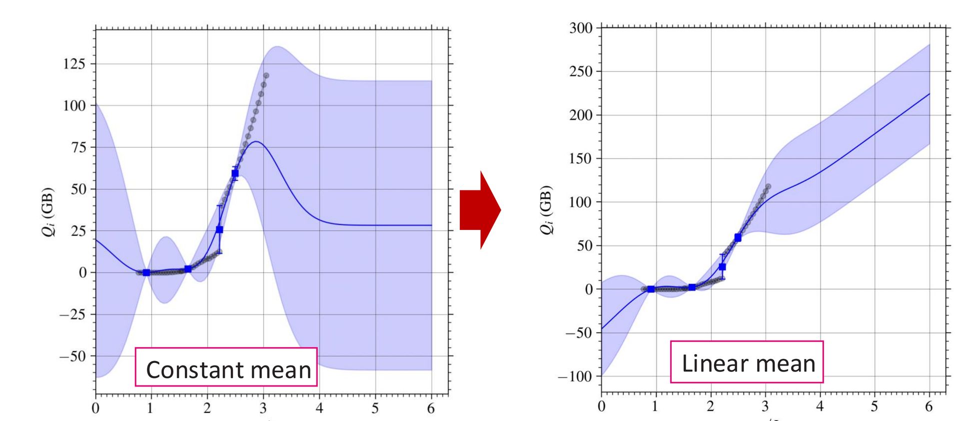
- Uncertainty quantification of flux evaluations is important to achieve fast convergence.

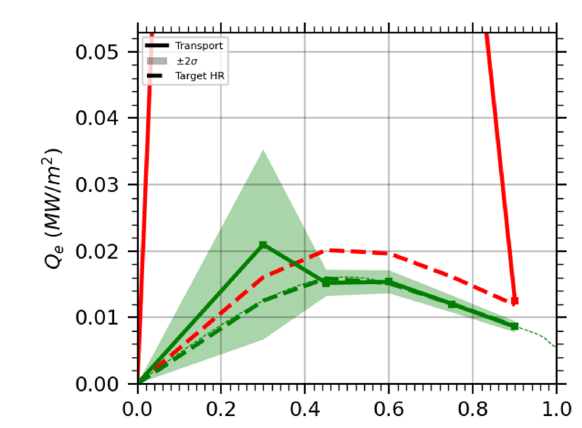






- At the expense of more evaluations per iteration, smoother convergence (as in [6]) and better stopping criteria reduce wall-time cost.
- Enforcing **positive-slope linear-mean** GP for diagonal terms of transport matrix → enforcing $Q_i \to \beta_{>0}\cdot a/L_{Ti}$ far from training ranges.

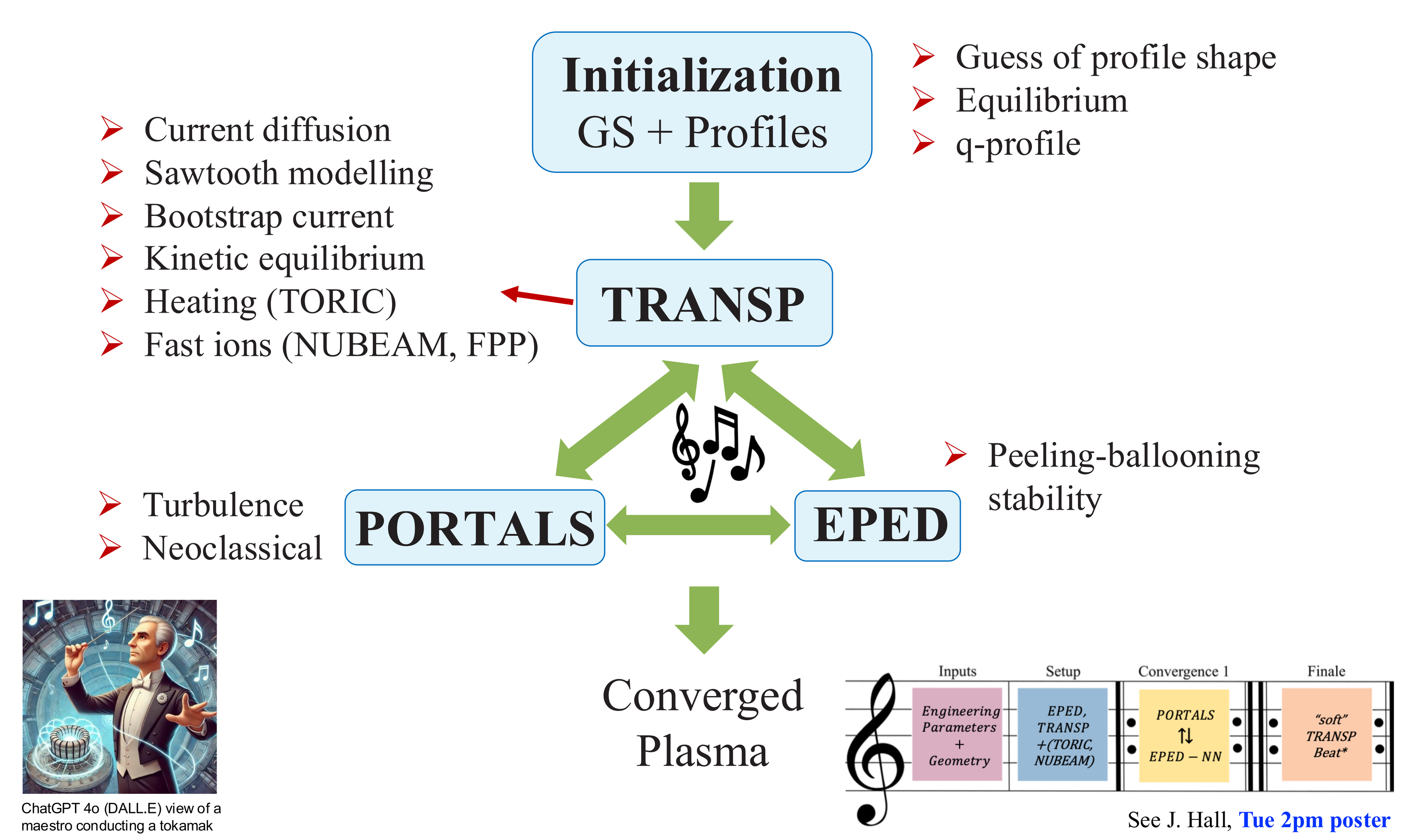




3. INTEGRATED MODELING WITH NEW MAESTRO WORKFLOW

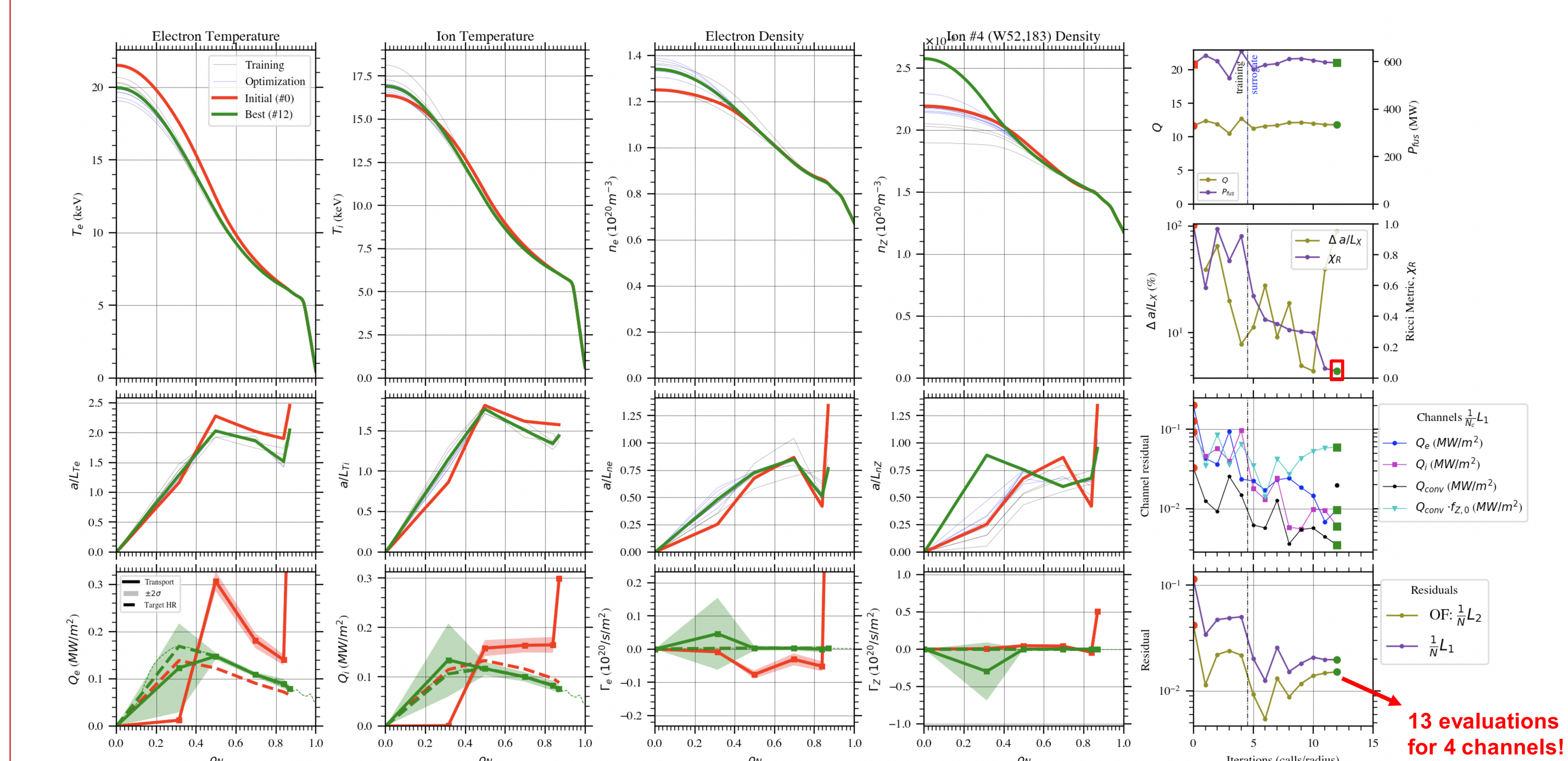
- Evaluating changes in equilibrium (e.g. q-profile, Λ_{shaf}), heating (e.g. Ohmic power, RF species partition and peak location) and edge boundary condition (e.g. β_N affecting p_{top}, w_{top}) is important for self-consistent plasma modeling.
- Similar to OMFIT STEP [7], MAESTRO loops over simulation codes (in *beats*) until self-consistent solution is found with PORTALS, EPED NN [2, J. Hall **Tue 2pm poster**], TRANSP [3] and FreeGS [8].

MAESTRO (**M**odular and **A**ccelerated **E**ngine for **S**imulation of **T**ransport and **R**eactor **O**ptimization)

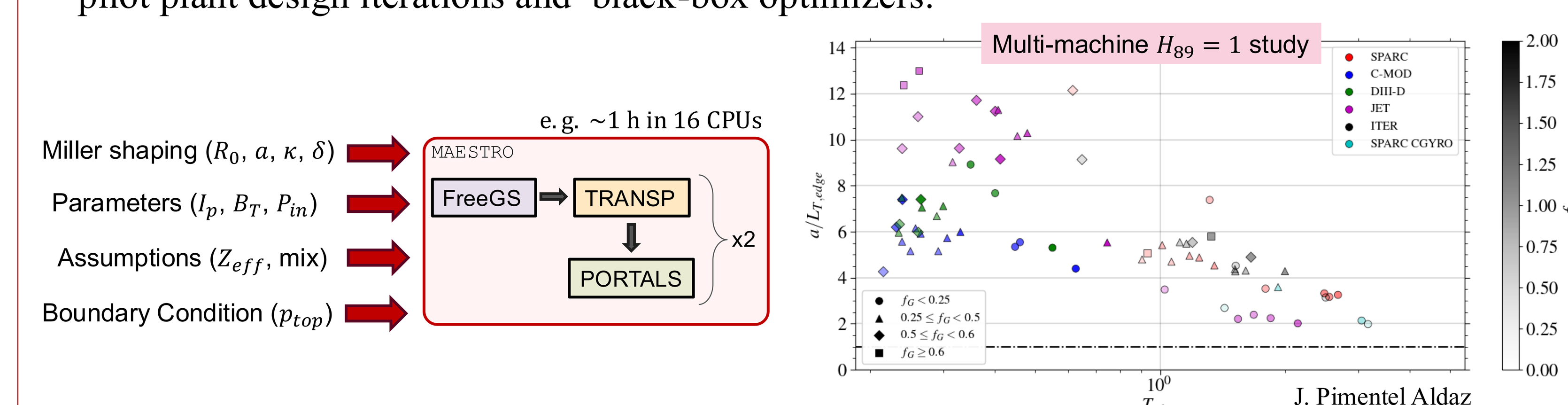


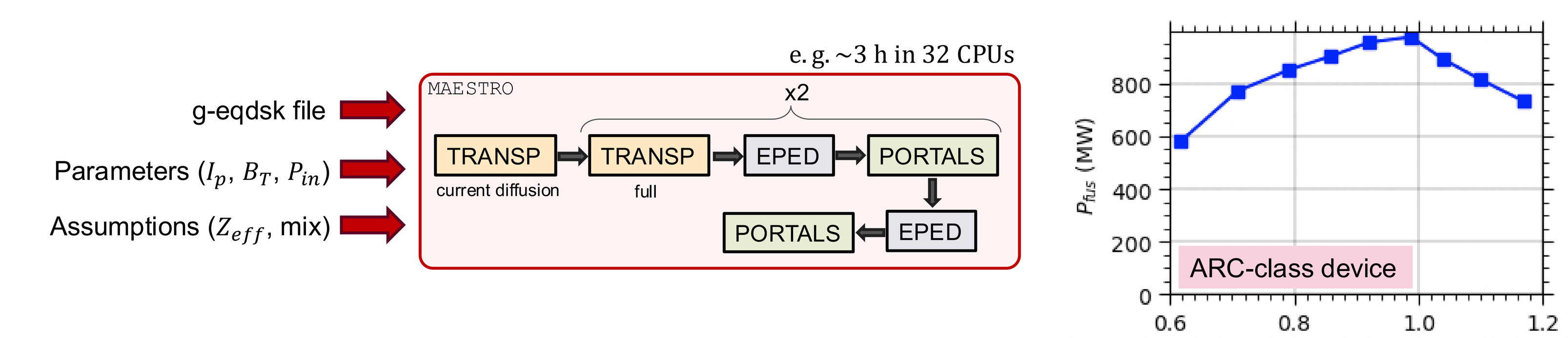
4. FROM ENGINEERING PARAMETERS TO PLASMA

- Multi-channel flux-matching solutions using full TGLF [4] with PORTALS are now achieved with just a few iterations and minimal user input.



- This enables full MAESTRO solutions at low cost, to be used in database studies, fusion pilot plant design iterations and black-box optimizers.





- Black-box nature of MAESTRO makes it suitable for Bayesian Optimization applications for device design [A. Saltzman PhD work, **Tue 10.30am session**].

4. CONCLUSIONS

- Surrogate–based optimization designed for expensive black-boxes very suitable for transport solvers → predictions possible with NL GK in PORTALS [1].
- Refinements to PORTALS techniques resulted in efficient solutions with quasilinear models like TGLF [4], even in the presence of discontinuities.
- MAESTRO developed to couple PORTALS with equilibrium, current diffusion, heating and pedestal models, providing self-consistent solutions at low cost and minimal user input.
- Using a "*from engineering parameters to plasma*" approach, MAESTRO enables extensive parameter studies, implementation within black-box optimizers, and fast iteration in fusion pilot plant design studies.

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