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Advanced algorithms for uncertainty quantification in plasma edge simulation chains

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Introduction and motivation

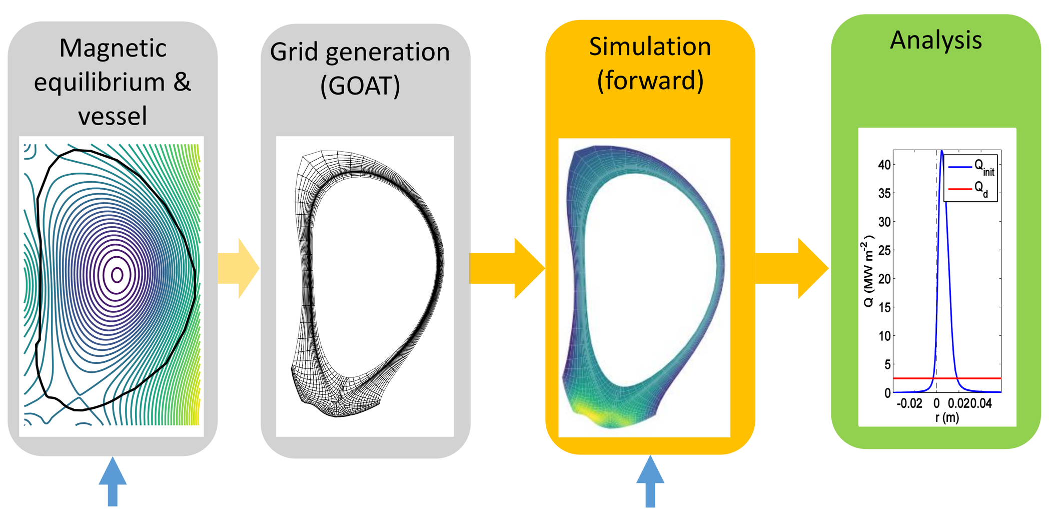
- Plasma boundary simulation tools are essential for interpretation of experiments and design of operational scenarios, yet are subject to significant model assumptions and uncertainties
- Uncertainty quantification (UQ) is often done on an ad-hoc basis since a reliable and robust UQ framework is missing
- The aim of this project is to provide a computationally efficient framework for uncertainty quantification and propagation using state-of-the-art plasma edge simulation codes such as SOLPS -ITER

Project overview

Goal: framework for UQ for state-of the-art plasma edge simulation chains

- Develop algorithms for **efficient** uncertainty propagation and model calibration for plasma edge codes
- Realize suitable workflow integration to automatically include magnetic equilibrium and grid generation in UQ
- **Assessment of dominant parameter uncertainties** for two key plasma-edge model validation uncertainties: 1) anomalous transport, and 2) magnetic equilibrium

Plasma edge simulation chain



Many uncertainties! Impact??

Approach

Algorithms for efficient UQ in plasma edge codes → Efficient workflow for UQ in plasma edge + magnetic equilibrium → Applications

Algorithms for efficient UQ in plasma edge codes
- Develop efficient forward UQ and model calibration
- Develop first framework for UQ at plasma-edge code level

Efficient workflow for UQ in plasma edge + magnetic equilibrium
- Single workflow for equilibrium reconstruction, grid generation, and plasma edge simulation
- Propagation of sensitivities through the code chain

Applications
- Impact of anomalous transport assumption on plasma edge model validation + assess different models
- Impact of magnetic field uncertainties
- Both effects together

Expected outcomes and milestones

- Integrated workflow for equilibrium simulation, gridding, and plasma edge simulations, including sensitivity propagation
- Forward UQ and model calibration framework for plasma edge codes
- Framework tested on different COMPASS cases

Transferable to

- Workflow can be used for validation efforts in WPs of EUROfusion programme (WPTE, WPPWIE, WPW7X) and associated TSVV tasks
- Algorithms can be applied to other (edge) codes
- The automated workflow and sensitivities can be used for magnetic field optimization [3] and paves the way towards robust design methods
- Framework can be used to calibrate and compare models in EnR on reduced turbulence transport models by Maurizio Giacomin
- Complementary to EnR of A. Jaervinen for edge/pedestal UQ

References

[1] Carli, S., et al. (2022), CTPP 62, e202100184
[2] Van den Kerkhof, S., et al. (2024), CTPP 64(7-8), e202300134
[3] Blommaert, M., et al. (2015), Journal of Nucl. Mat., 1220-1224

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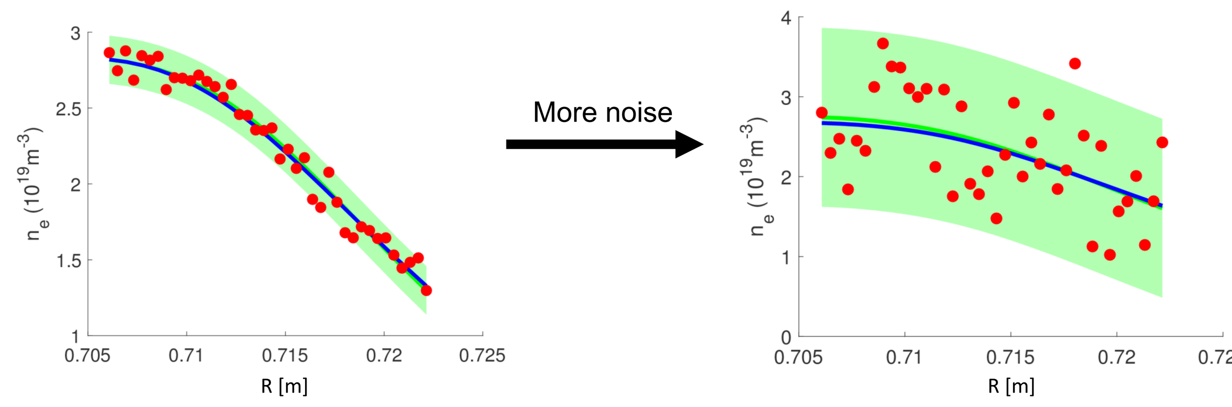
Development of advanced UQ algorithms

Challenges:
- Possibly many inputs/outputs
- Requires automated workflow
- Forward UQ and backward UQ (model calibration) for computationally intensive code

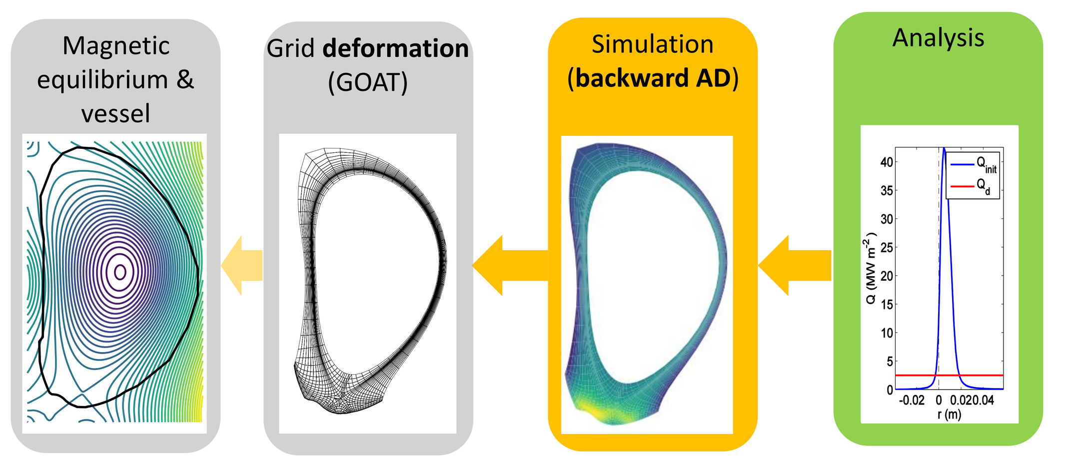
Solutions:
- FUQ: add sensitivity info to basic methods, MLMC
- BUQ: Speed-up via one-shot, hybrid multilevel for global optimum, Markov chain MC
- Alternative: surrogate approximation of posterior distribution by, e.g., Gaussian process
- For SOLPS: starting point AD framework of S. Carli [1], MAP for synthetic data



Sensitivity computation in multi-physics workflows

Options:
- Finite differences: easy, but truncation error & cost proportional to # inputs
- Algorithmic Differentiation: accurate, but requires access to all source code simultaneously
- Adjoint: most efficient, but requires manual implementation of Jacobian

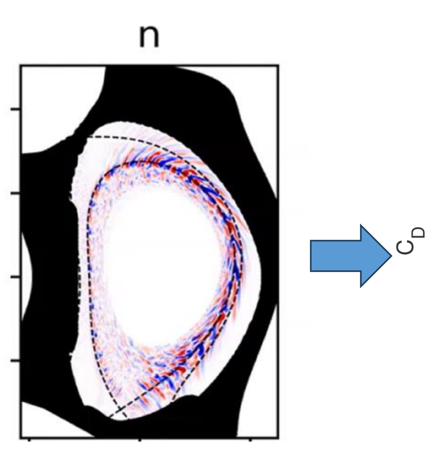
→ Here: **taylored approach**



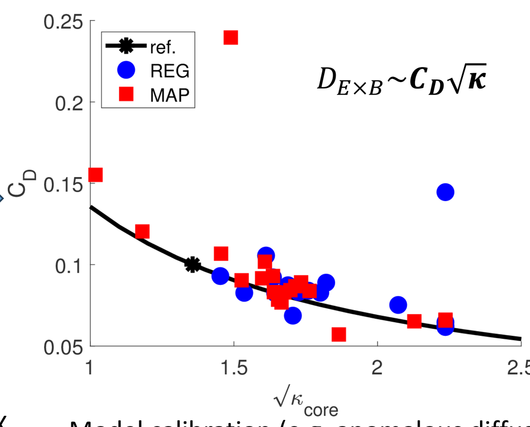
Specific outcome from applications

Using the UQ framework, we will provide an answer to the following questions:
- What is the model error made by anomalous transport models?
- How do different anomalous models perform?
- What is the impact of magnetic field uncertainties on midplane profiles?
- How do both uncertainties impact target heat and particle flux profiles?

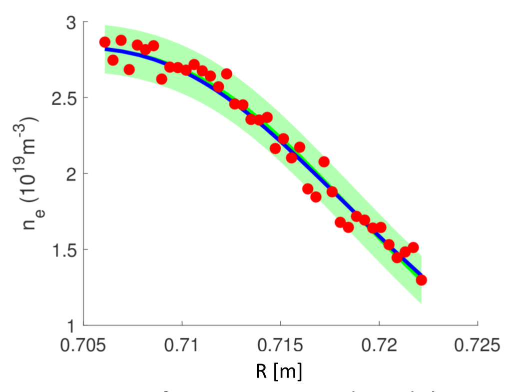
Case studies on COMPASS, but naturally extendable to any device or scenario



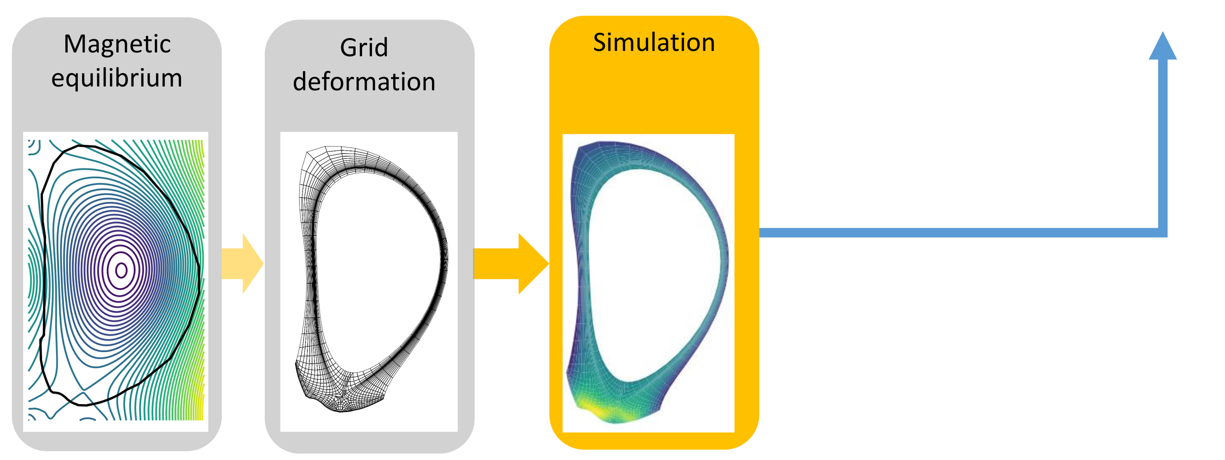
Turbulence data from SOLEDGE3X



Model calibration (e.g. anomalous diffusion) and input uncertainty quantification



Impact of uncertainty and model error on target and midplane profiles



Uncertainty on magnetic equilibrium, propagated through plasma edge code with sensitivities