KU LEUVEN

Summary and discussion
Topic C: FHK, AD, UQ

FHK modeling based on AFN

- AFN models and hybrid methods (in particular, SpH) reached high level of maturity
  - Including effects of drifts, molecules, n-n collisions,…
  - Coupling with impurity models
- Integration in various codes
  - Default models in SOLPS-ITER extended grids version. Relevant input files automatically generated.
  - Basic AFN models implemented in various European turbulence codes (link TSVV3), incl. SOLEDGE3X, GRILLIX
- Already applied to simulate multiple machines, incl. TCV, AUG, JET, ITER, DEMO (link WP TE, WP DES)
- Next steps
  - Validation n-n collision effects with kinetic simulations
  - Extension to ‘hydrodynamic’ closure model for void regions w/o plasma
  - Fluid model for molecules?

FHK modeling based on KDMC

- Basic particle tracing scheme implemented in EIRON
- Estimation of QoIs through fluid model based on particle positions
  - Proof and 1D demonstration available, for homogeneous background
- Next steps
  - Extension to heterogeneous background
  - Integration of estimators in EIRON
  - Integartion with multi-level scheme

AD, UQ

- Derivatives based on AD (TAPENADE) in forward mode available
  - EIRENE standalone
- UQ demonstration: applied to study sensitivity of QoIs to uncertainty in reaction rate coefficients
  - Accurate in low/medium recycling regimes
  - Problem of diverging derivatives in high recycling regimes
- Next steps
  - Analysis of derivative problems in high recycling
  - Analysis of impact estimators on accuracy of derivatives
  - Implementation adjoint AD with TAPENADE
  - Adjoint differentiation of couple B2.5-EIRENE solver
- Potential for building implicit coupling to plasma codes (B2.5, SOLEDGE3X) and providing sensitivities (ERO2.0)