

# **Overview of ERO2.0 and interactions with EIRENE**

#### J. Romazanov on behalf of the ERO Developer Team

Forschungszentrum Jülich GmbH, Institute of Fusion Energy and Nuclear Waste Management - Plasma Physics (IFN-1), 52425 Jülich, Germany



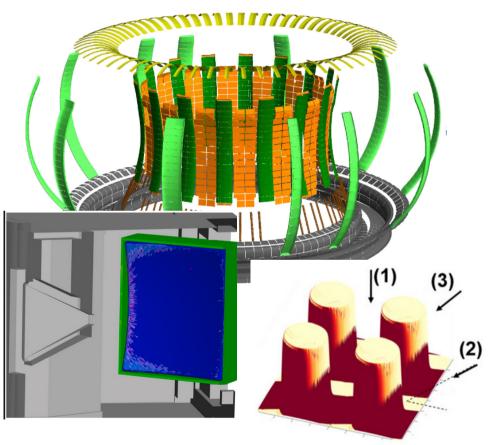
# **Overview of the code**



#### **Key facts**

- Core developer team at FZJ + international collaborations
- Monte-Carlo code for PWI (erosion, deposition) and impurity transport code
- Detailed, fully 3D (CAD-based) wall geometry
- Possibility of Larmor-resolved ion orbits
- Written in C++ (modular, object-oriented)
- MPI + OpenMP parallelization, GPU acceleration in work
- Interfaces to other codes

#### Macro and micro geometries in ERO2.0

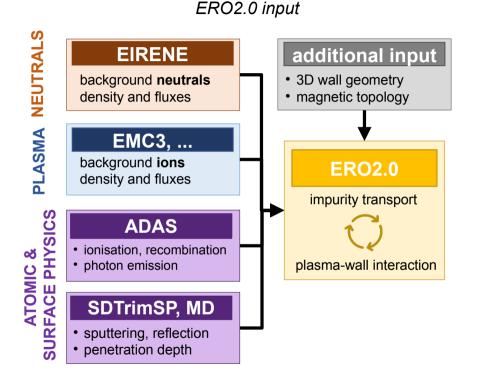


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# **Examples of ERO2.0 applications**

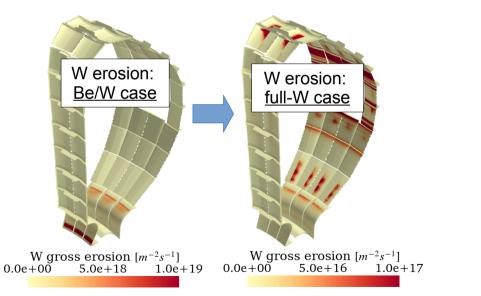


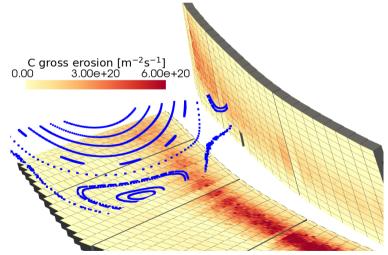
#### **ITER tokamak**

- Be wall lifetime considering 3D shaping
- diagnostic first mirrors lifetime
- transition from Be to W first wall

#### W7-X stellarator

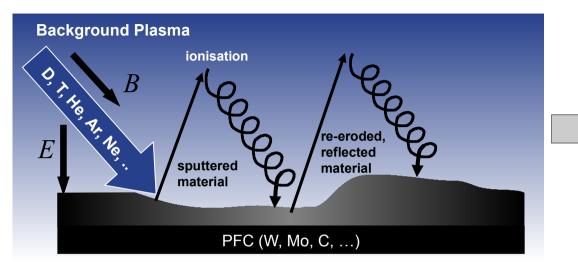
- graphite (carbon) erosion
- impurity transport in 3D environment
- long-pulse operation, upgrade to metallic wall





# **Key physics included**





## **Basic output:**

- Erosion/deposition patterns on the wall
- Distribution of impurities in the plasma

#### **Plasma-wall interaction**

- physical and chemical sputtering
- reflection
- material mixing
- re-erosion, re-deposition

#### **Impurity transport**

- ionisation, recombination, dissociation of molecules
- Full Orbit or Guiding Center
- collisions (Fokker-Planck) in trace impurity approximation

[1] Kirschner et al., NF(2000)[2] Romazanov et al.,Phys. Scr. (2017)

# **Overview of ERO2.0** $\leftrightarrow$ **EIRENE interaction topics**



- Databases (A&M, PWI)
- Simulation data exchange
- Kinetic ion transport model
- Software engineering
- Others (e.g. code coupling)

# Interactions ERO2.0 o EIRENE: A&M database



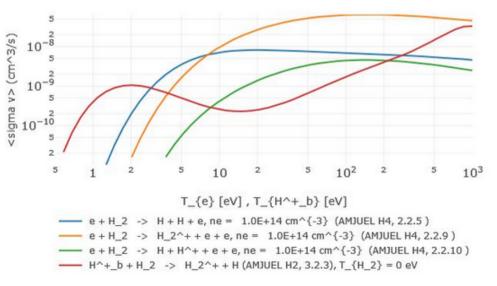
### • ADAS data

- ionisation/recombination, photon emissivities
- Molecular data
  - ERO2.0: focus on impurities (hydrocarbons, N2, ammonia, ..)
  - EIRENE has much more comprehensive model & data incl. hydrogen molecules
- Possible actions:
  - Build common curated database
  - Coupling to ModCR

<u>Linked projects:</u> TSVV-5, ...

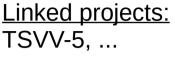
# from EIRENE webpage

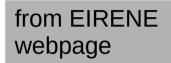
#### H2 dissociation rate coefficients



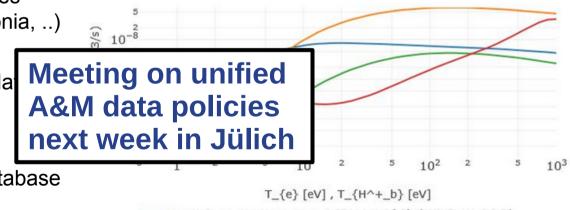
Interactions ERO2.0 ↔ EIRENE: A&M database

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H2 dissociation rate coefficients



- ----- e + H\_2 -> H + H + e, ne = 1.0E+14 cm^{-3} (AMJUEL H4, 2.2.5)
- e + H\_2 -> H\_2^+ + e + e, ne = 1.0E+14 cm^{-3} (AMJUEL H4, 2.2.9)
  - e + H\_2 -> H + H^+ + e + e, ne = 1.0E+14 cm^{-3} (AMJUEL H4, 2.2.10)
- H^+\_b + H\_2 -> H\_2^+ + H (AMJUEL H2, 3.2.3), T\_{H\_2} = 0 eV



# Interactions ERO2.0 o EIRENE: PWI database

**JÜLICH** Forschungszentrum

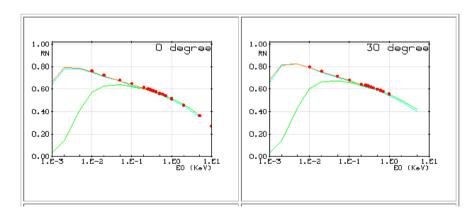
- Reflection coefficients
  - typically from TRIM (SDTrimSP)
  - same data layout needed (function of e.g. impact energy and angle)
  - ERO2.0 also uses sputtering coefficients (from same simulations)
- Possible actions:
  - Build common curated database
  - Requires streamlining of formats and review of input parameters / assumptions
  - Integrate MD data?

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<u>Linked projects:</u>
TSVV-7, ...
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# from EIRENE webpage

#### **Particle Reflection Coefficient**

D on W



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Interactions ERO2.0 o EIRENE: simulation data exchange

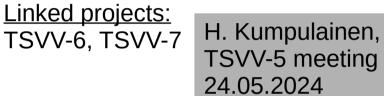
# • X-EIRENE input to ERO2.0:

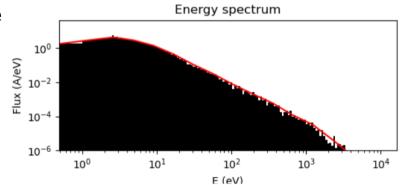
- charge-exchange neutrals: energy and angular resolved fluxes for calculation of erosion
- volumetric data: neutral densities and temperatures for impurity collisions

Possible actions:

- Define prioritised "common interest" plasma cases. Ensure plasma backgrounds are suitable for ERO2.0.
  - Example: SOLPS-ITER cases for ITER, DEMO: often outdated or wrong wall geometry/equilibrium, no wide-grid, no CXN data, ...
- Streamline exchange on common grids (ERO2.0 M.Sc. thesis in progress) j.romazanov@fz-juelich.de | EIRENE-NGM Code Camp 2024, DIFFER

\*(EIRENE coupled to B2, EMC3, SOLEDGE, ..)







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# Interactions ERO2.0 in EIRENE: simulation data exchange

# • X-EIRENE input to ERO2.0:

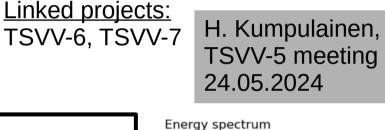
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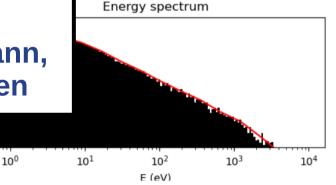
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# Interactions ERO2.0 Heta EIRENE: kinetic ion transport model

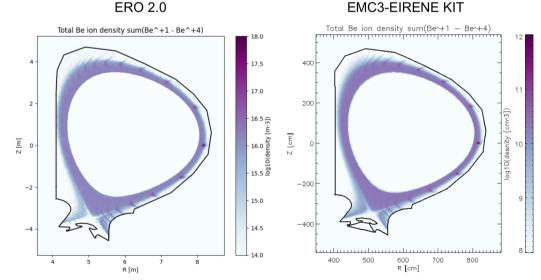


## • EIRENE Kinetic Ion Transport (KIT)

- same equations as for ion transport in ERO2.0
- Possible actions:
  - Code-code benchmark
  - Streamline and imporove technical implementation (e.g. adaptive stepping)
  - Comparison Guiding Center vs Full-Orbit
  - Implement higher-order corrections (thermoforce, ...)
  - Non-linear effects?

Linked projects: TSVV-6, ...

# D. Harting, PSI-26



# 

- EUROfusion Standard Software recommendations:
  - IMAS interfaces 0
  - software engineering best 0 practises (CI/CD, documentation, issue tracker, code webpage, ...)
  - licensing 0
  - training 0
  - validation & verification 0
- Possible actions:
  - Share know-how, streamline as 0 much as possible (shared infrastructure etc.)

Linked projects: TSVV-5. TSVV-6. TSVV-7



Annex-2 Guidelines for EUROfusion standard software

#### Gitlab server @FZJ:



EIRENE / EIRENE 🔂 Developer



A Monte Carlo transport solver: multi species, nonlinear and time dependent. See also http://www.eirene.de Monte Carlo neutral gas ... plasma physics



ero / ero2 🔒 Owner ERO2.0 source code + master config file.



# Interactions ERO2.0 Heta EIRENE: other topics



- Parallelisation
  - Both codes use MPI + OpenMP -> exchange on ideas for profiling, optimisation, GPU acceleration, ...?
- Data storage
  - SimDB being built for X-EIRENE simulation data -> cousage by ERO2.0?
- Code-code coupling
  - Implement "real coupling" between ERO2.0 and X-EIRENE? (ERO2.0 providing impurities)

Linked projects: TSVV-5, TSVV-6, TSVV-7