Status and prospects of ERO2.0 activities relevant to TSVV-7

J. Romazanov, on behalf of the ERO2.0 team

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Outline

- Introduction to the ERO2.0 code
- Application to ITER as proxy for DEMO
- Studies on erosion of rough surfaces
- Embedment of ERO2.0 in TSVV-7
- Overview of planned developments

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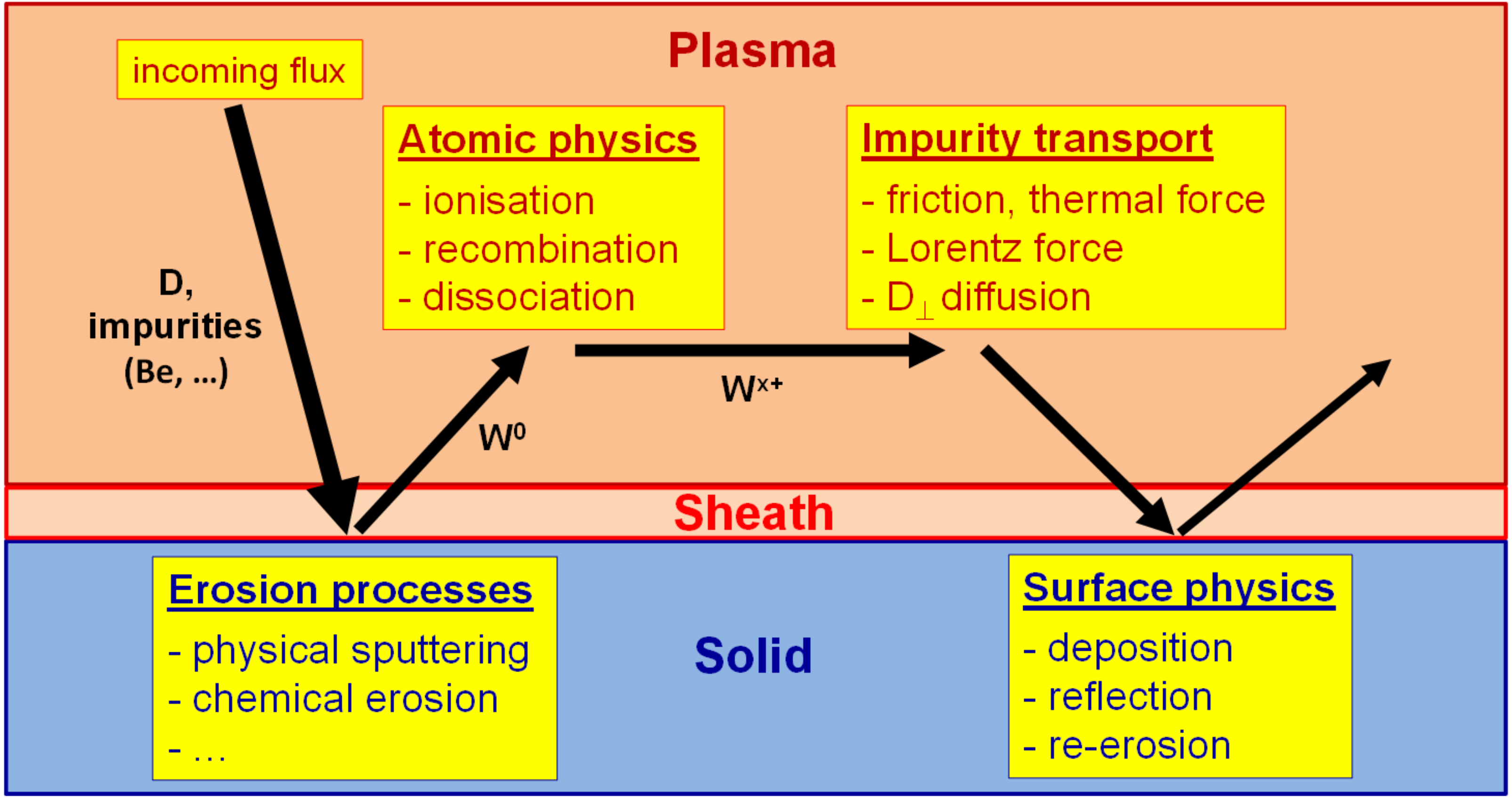
Introduction to the ERO2.0 code



Plasma

incoming flux

D, impurities (Be, ...)

Atomic physics

- ionisation
- recombination
- dissociation

Impurity transport

- friction, thermal force
- Lorentz force
- $D_\perp$ diffusion

W^0

W^{x+}

Sheath

Erosion processes

- physical sputtering
- chemical erosion
- …

Solid

Surface physics

- deposition
- reflection
- re-erosion

Components of the ERO2.0 model

(1) Wall geometry model

- polygon mesh + material distribution

(2) Background plasma model

- constant input plasma background (n_e, T_e, T_i, $v_{||}$, E, B)
- imported from edge plasma codes (SOLPS-ITER, EMC3-EIRENE, …)
- shadowing correction (based on 3D magnetic field line tracing)

(3) PMI model

- sputtering yields & reflection coefficients → imported from BCA & MD codes + assumptions about impact distributions
- assumptions on the initial surface roughness
- material mixing model → homogeneous mixing (HMM)

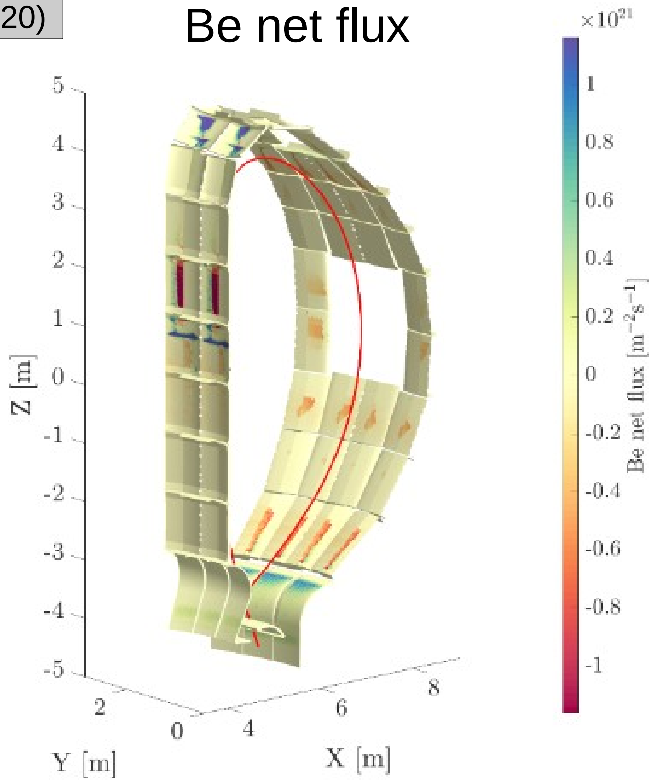
(4) Transport model

- test particle trajectories (solutions of Fokker-Planck equation)
- atomic data (ionisation & recombination rates, photon efficiencies) from ADAS

Application to ITER: erosion of the First Wall (FW)

J. Romazanov et al.,
Contrib. Plasma Phys. (2020)

- **Input:**
  - 2D plasma background from OEDGE (SOLPS + extended grid by onion-skin model)
  - 3D wall geometry: 20° toroidal sector + periodic boundaries
- **ERO2.0 modelling:**
  - Beryllium (Be) steady-state erosion due to D ions, D CX neutrals, Be self-sputtering
  - One of the important outputs is Be net erosion (deposition minus erosion) which is relevant for lifetime predictions
  - Typical net erosion fluxes are ~10^{21} Be/m²/s (gross erosion is ~10 times higher)
  - About 10% of Be migrates to the divertor, 90% stays in main chamber
  - Study was extended to various plasma conditions and to scan other simulation parameters (e.g. background particle impact angle)



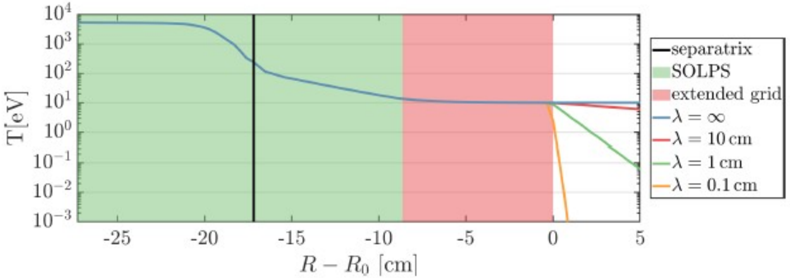
🟥 net erosion

🟦 net deposition

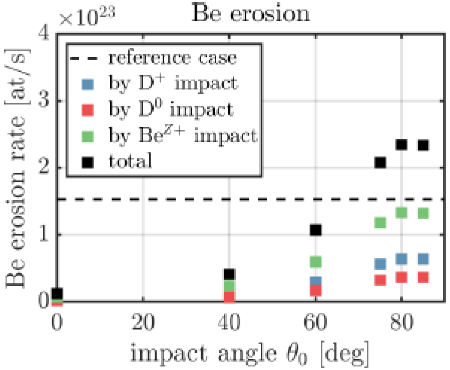
Typical model uncertainties

J. Romazanov et al.,
presented at PSI (2021)

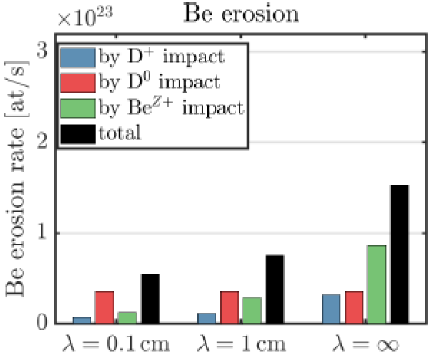
- **Impact angle distributions:**
  - Known only for particles “tracked” by ERO2.0! (here: Be)
  - For “background particles” (here: D) needs simplified assumptions (e.g. constant impact angle) or importing from other codes (e.g. EIRENE → CX, PIC → ions)
  - Can change erosion by an order of magnitude!
  - Affected by surface roughness (more on this later)
- **Plasma parameters at surface:**
  - E.g. plasma flux, temperature
  - Extrapolation needed due to grid gap of SOLPS



Influence of D impact angle



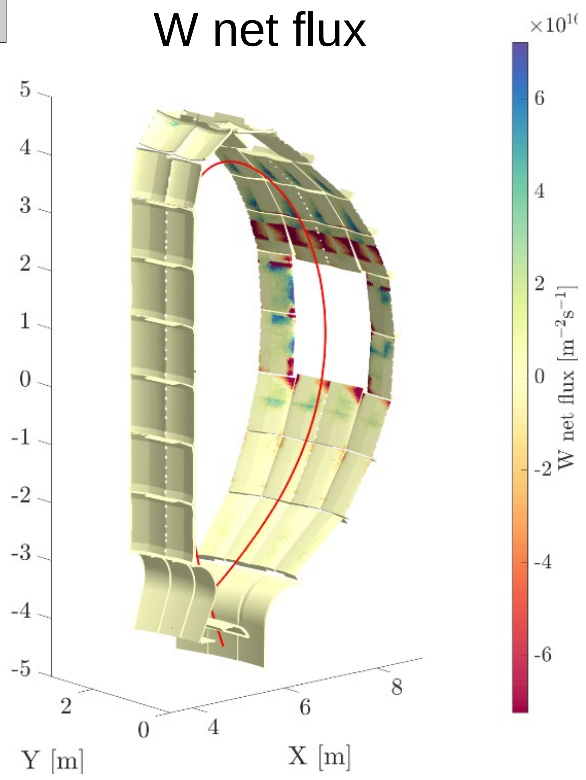
Influence of plasma BG extrapolation



Parameter study: ITER with full-tungsten wall

A. Eksaeva et al.,
presented at PFMC (2021)

- **Background:**
  - DEMO needed predictions of W erosion/deposition to assess wall lifetime, retention, dust production
  - No suitable wall description or plasma backgrounds were available → used ITER as a proxy
- **Results:**
  - Overall main wall erosion much smaller compared to Be wall (factor ~10^4)
  - W sputtering at main wall only due to D CX neutrals and self-sputtering
  - 99% of sputtered W at main re-deposited at main wall (or gaps at main wall), 1% flows to divertor
  - Study was extended to different magnetic configurations and seeding impurities (Kr, Ar, Ne, Xe) at various concentrations



🟥 net erosion
🟦 net deposition

Roughness: introduction

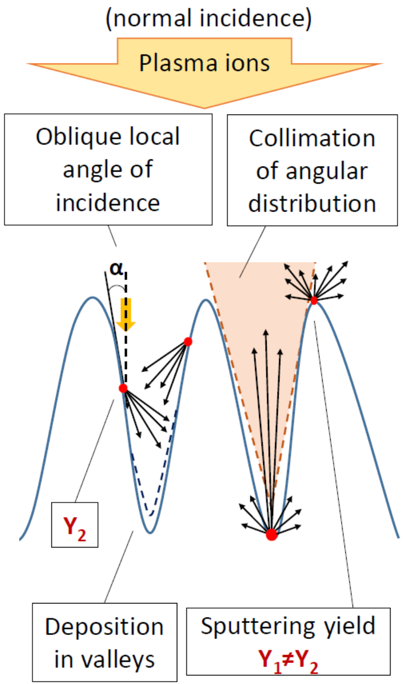
- Micro-scale surface roughness exists from sample preparation
- Roughening during plasma exposure observed for some samples (cones, needles, fuzz)
- Surface roughness has several effects on erosion:
  - Immediate redeposition of sputtered atoms inside the structures
    - Reduces sputtering yield
    - Collimates sputtered angular distribution
  - Incoming angular distribution different from a flat surface

ERO2.0 simulations on a micro-scale with arbitrarily shaped, pre-defined rough surfaces are possible

Initial rough surfaces must be pre-defined (AFM/SEM measurements or analytical shapes → somewhat arbitrary)

Alina Eksaeva, dissertation (2020)

Illustration of surface roughness effects on erosion



(normal incidence)

Plasma ions

Oblique local angle of incidence

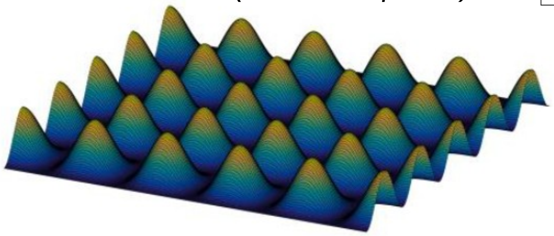
Collimation of angular distribution

Y_2

Deposition in valleys

Sputtering yield $Y_1 \neq Y_2$

Example of pre-defined regular surface in ERO2.0 (3D cosine peaks)

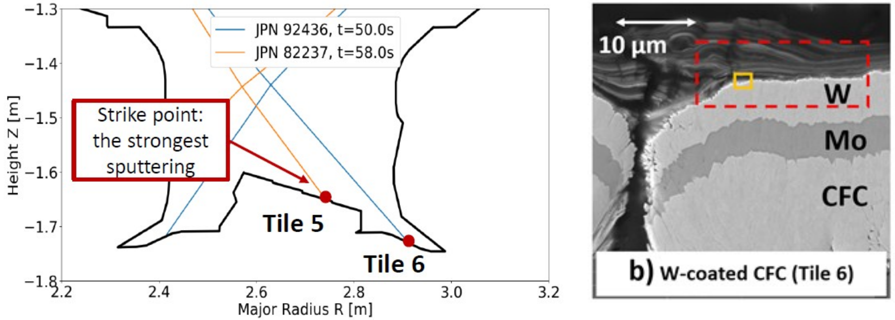


Roughness: application to JET

A. Eksaeva, JNME (2021)

- Post-mortem analysis shows:
  - Tile 6 has ~2x larger roughness than tile 5
  - Tile 6 also has~2x lower net erosion rate → causality?
- Micro-scale simulations performed with different rough surfaces
  - randomly generated fractal surfaces
  - regular cosine peak surfaces

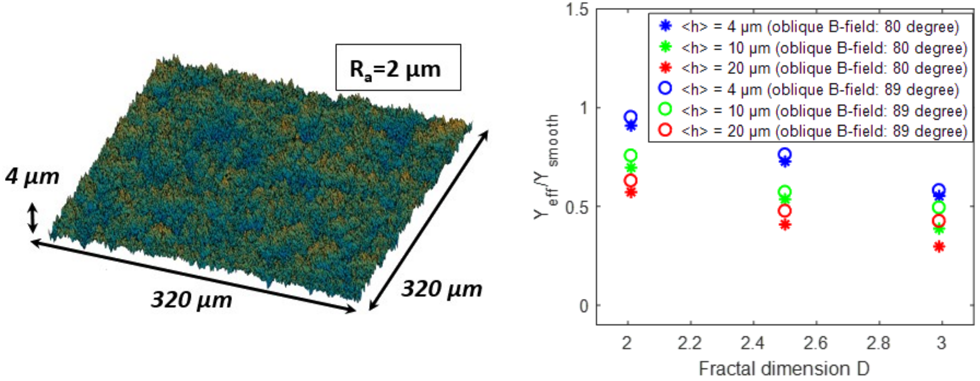
JET divertor and post-mortem analysis



Simulations confirm that roughness may explain the factor ~2 difference in erosion from different JET W divertor regions

More detailed studies needed to understand origin of roughness, and rule out other possible reasons (e.g. same plasma parameters were assumed for Tile 5 and 6)

Example of ERO2.0 simulations with assumed fractal surfaces



Evolution of rough surfaces

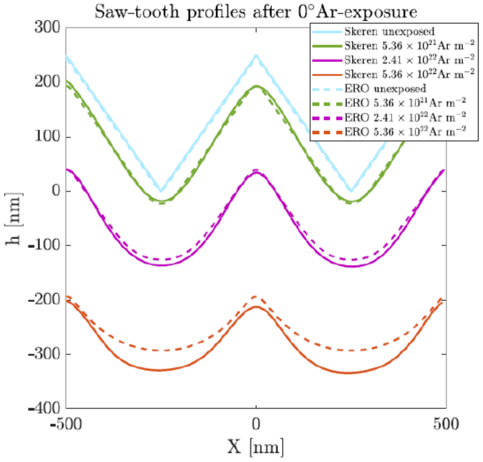
G. Alberti et al, PFMC conference (2021)
G. Alberti et al, Nucl. Fusion (2021)

- **Comparison with analytic Skeren model:**
  - Reasonable agreement shown for W surface evolution
  - But: smoothing algorithm in ERO2.0 leads to overestimated surface smoothing in the long run.
- **Influence of grains:**
  - ERO2.0 model does not include grains, but Skeren model does. What is the possible influence of grains?
  - Larger grains → roughening, compared to single-crystal solution

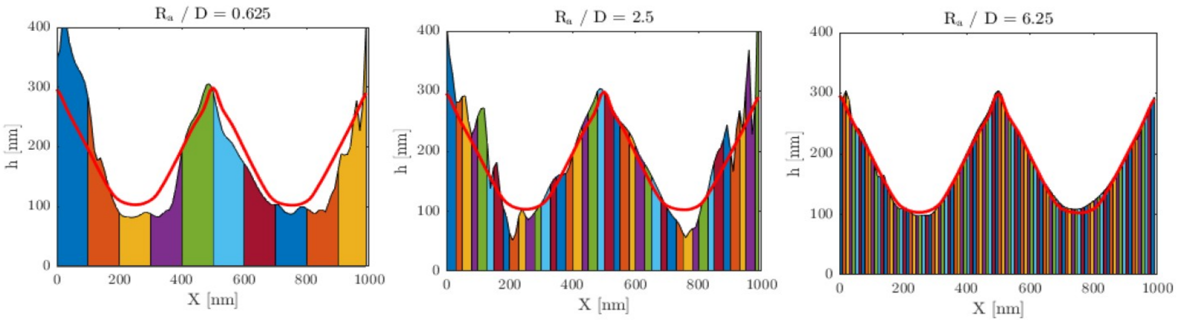
Skeren model

$$\frac{\partial h}{\partial t} = \underbrace{-\Omega\Gamma\frac{\cos\varphi}{\cos\phi}Y\left(E,\varphi\right)G\left(x,y\right)}_{\text{erosion term}}\underbrace{-\mathbf{K}\Omega\Gamma\cos\varphi\Delta^2 h}_{\text{diffusion term}}$$

ERO2.0 vs Skeren: W roughness evolution



Influence of grain size



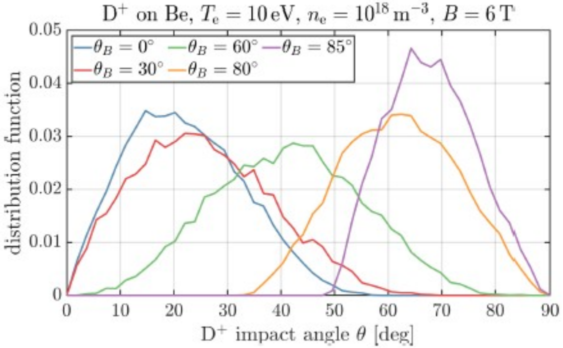
Connection to EUROfusion grant on Machine Learning methods

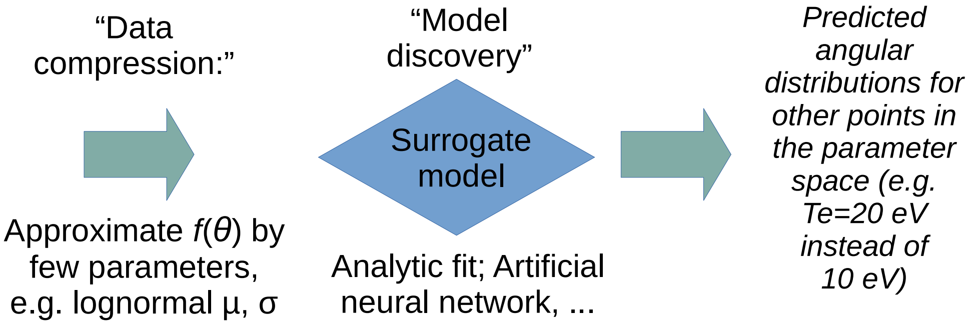
Development of machine learning methods and integration of surrogate model predictor schemes for plasma-exhaust and PWI in fusion

Project leader: Sven Wiesen

- EnR sub-project 3: “Model discovery for erosion yields through ML methods”
- Example: influence of background particles impact angle distribution
  - Method 1: set to some reasonable constant value (e.g. 0°, 60°, ...)
  - **Method 2**: create distributions f(θ) database with the aid of ML:
    - magnetic field strength and inclination angle
    - sheath properties (ne, Te, Zeff, …)
    - roughness
- TSVV-7 can create DEMO-relevant “training set” for EnR

Example of numerical angular f(θ) distributions for different magnetic field angles.





“Data compression:”

Approximate *f*(*θ*) by few parameters, e.g. lognormal μ, σ

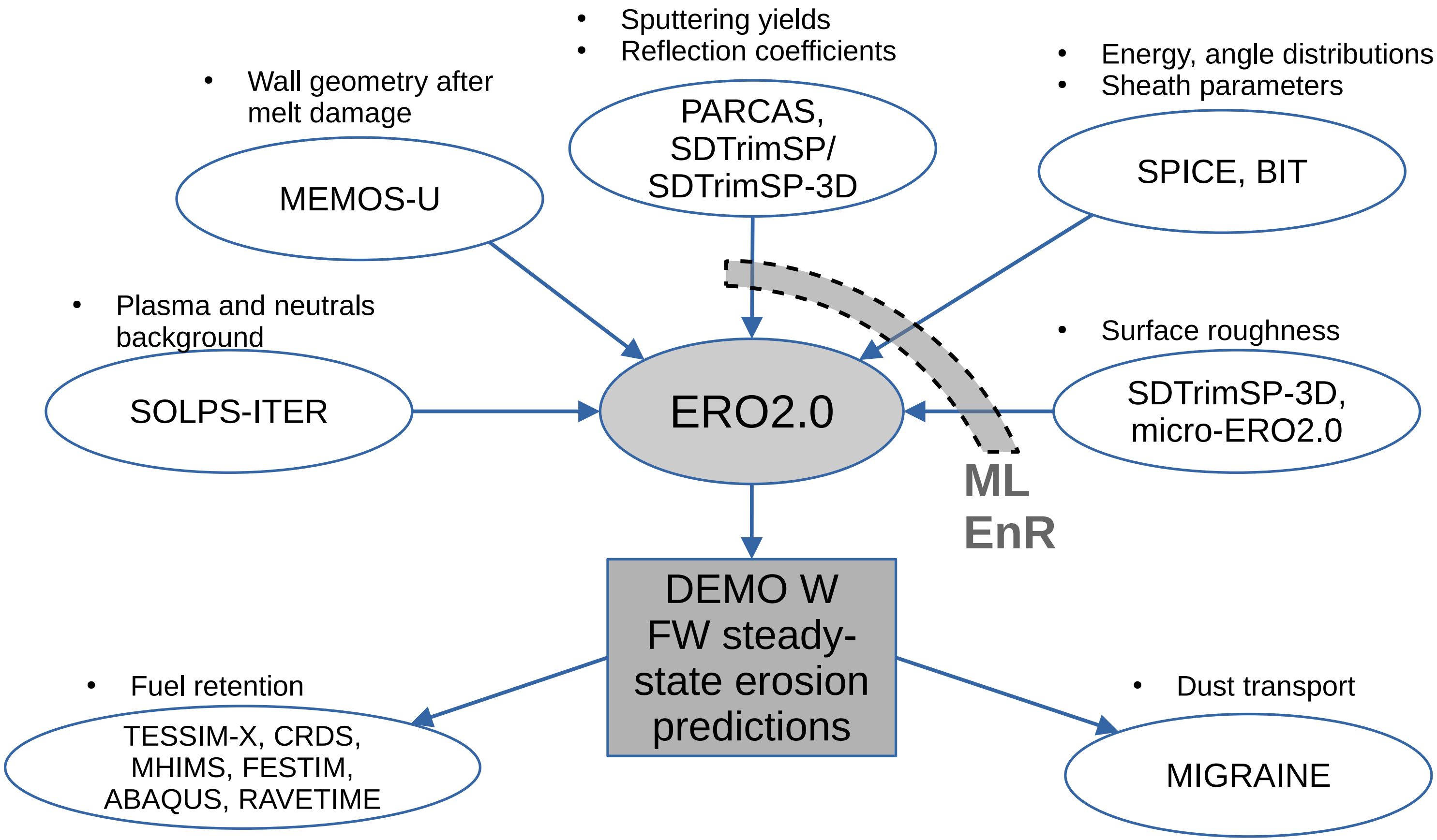
“Model discovery”

Surrogate model

Analytic fit; Artificial neural network, ...

Predicted angular distributions for other points in the parameter space (e.g. Te=20 eV instead of 10 eV)

Flowchart: data flow to and from ERO2.0 in TSVV-7



- Sputtering yields
- Reflection coefficients

PARCAS, SDTrimSP/ SDTrimSP-3D

- Wall geometry after melt damage

MEMOS-U

- Energy, angle distributions
- Sheath parameters

SPICE, BIT

- Plasma and neutrals background

SOLPS-ITER

ERO2.0

- Surface roughness

SDTrimSP-3D, micro-ERO2.0

ML
EnR

DEMO W FW steady-state erosion predictions

- Fuel retention

TESSIM-X, CRDS, MHIMS, FESTIM, ABAQUS, RAVETIME

- Dust transport

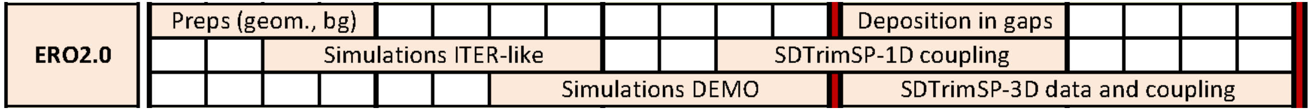
MIGRAINE

Manpower for TSVV-7 at FZJ

Postdoc position for ERO2.0 activities is now tendered!

Person-months at FZJ

		2021	2022	2023	2024	2025
Dmitry Matveev	Task leader; retention	6	6	6	6	6
Juri Romazanov	ERO2.0	0	0	6	6	6
Sebastian Rode	ERO2.0	6	9	6	6	6
NN (Postdoc)	(ERO2.0?)	6	6	6	6	6
Σ		18	21	24	24	24


ERO2.0

Preps (geom., bg)

Deposition in gaps

Simulations ITER-like

SDTrimSP-1D coupling

Simulations DEMO

SDTrimSP-3D data and coupling

Foreseen improvements of ERO2.0

Postdoc position for ERO2.0 activities is now tendered!

- **Model improvements:**
    - Importing spatially resolved background impurities (e.g. seeding species)
    - “Advanced mixing model” (depth resolution of material concentrations)
    - Spatially resolved anomalous diffusion coefficient for impurities
    - Feedback of impurities on the plasma (iterative scheme – “Tokar model”)
    - Improved core impurity transport (COREDIV coupling)
    - Improvement of micro-ERO2.0 roughness model (eliminate smoothing artifacts, consider grains)

OCPC started

- **Integrated modelling:**
    - Direct coupling to SDTrimSP (on-the-fly sputt. yields and reflection coeff., depth resolution)
    - Improved (automatic) coupling to SOLPS-ITER (or other transport codes) + iterative scheme
    - Direct coupling to CRDS (fuel content influences physical + chemical sputtering)
- **Others:**
    - IMAS compatibility
    - Improved MPI-OpenMP scheme; vectorization; GPU parallelization

ACH support needed