EUROfusion

E-TASC General Meeting #2

9-13 February 2026, Max Planck IPP

TSVV-K PI: D.V.Borodin (*d.borodin@fz-juelich.de*)

TSVV-K: Neutral Particle Models

TSVV-K team:

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General task deliverables

- **WP1 (call): Establish a multi-fidelity model hierarchy for the physics of neutrals, ranging from first principles models to reduced representations, and integrate it into fluid and gyrokinetic edge turbulence simulations. Exploit synergies with TSVV-B and TSVV-C.**
  - **WP1.1 Advanced fluid models - KUL**
  - **WP1.2: Improved Kinetic Diffusion Monte-Carlo (KDMC) - KUL + ACH-MPG**
  - **WP1.3 Interface to CFD codes - CAE/AMU+ ACH-IPPLM**
- **WP2 (call): Develop high fidelity collisional-radiative models for H, D, T neutrals further, apply them to mixed fuel plasmas, and assess properties of charge-exchange neutrals.**
  - **WP2.1 Development of ModCR and PLOUTOS – FZJ + DIFFER + ENEA**
  - **WP2.2 Validation with experiment, photon tracing and ColRad development Aalto + all**

WP0: Overall project management and code maintenance - FZJ

ACH support and other partners

- **ACH-IPPLM. IMASification** of EIRENE. For starters it was based on pre-existing B2.5 parallelization inside the SOLPS package, but it is going consequently more into the EIRENE itself; (EIRENE treats multiple grid types - we go GGD objects defined for SOLPS-related "triangles" to more generalized ones aimed to cover all of EIRENE cell types).
- **ACH-MPG. EIRON** "toy-model" – reduced down to skeleton of EIRENE special code for testing of various parallelization and domain decomposition schemes. Profiling and **parallelisation** (hybrid MPI/OpenMP) of EIRENE, code refactoring and streamlining was also profiting from the ACH support. We anticipate extension to KDMC optimisation.
- **Links with other TSVVs (in particular TSVV-B,C and D)** are under joint discussion, we do presentations at joint meetings incl. the code camps. The focuses are the **interfaces (based on STYX2.0)** between the codes as well as jointly defined **reference simulation cases**.
- Due to **SOLPS-ITER and other packages involving EIRENE** we maintain strong direct contact with **ITER**. The EIRENE repositories at FZJ and ITER are mirrored. The code **forking** was significant – now **reduced** down due to the recent "milestone version" **(MsV) release** in 2024. Still, further contributions from both sides are to be incorporated on routine basis. EIRENE database development is also of large interest for ITER.
- Work on **A&M databases** (also surface data) is supported by the **IAEA** AMD Unit (https://amdis.iaea.org/GNAMPP).

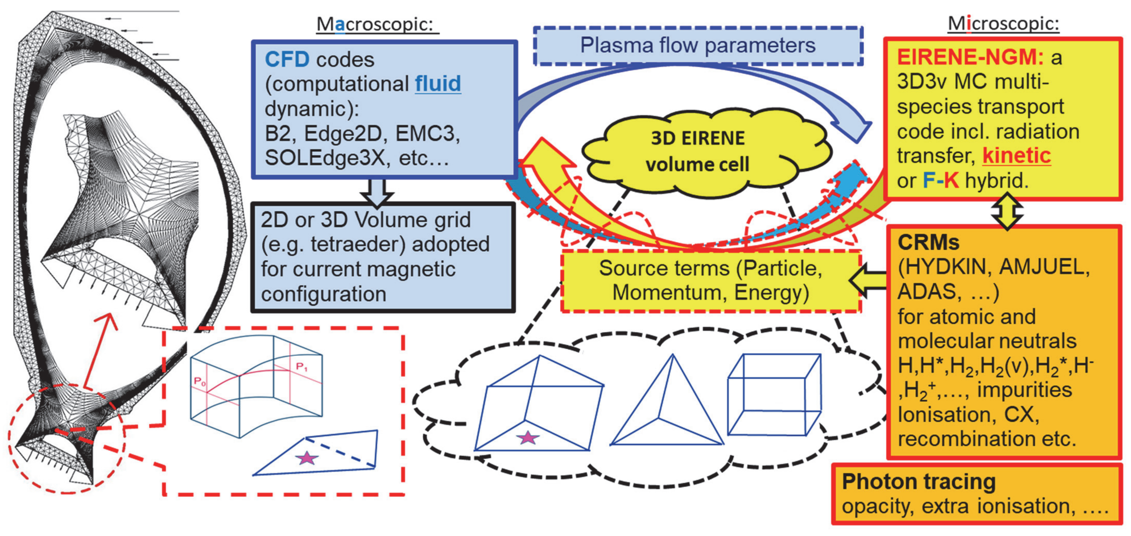
EIRENE-NGM package

EIRENE code

The EIRENE code [1][2] also known as Neutral Gas Module (NGM) is a **multi-purpose Boltzmann-equation Monte-Carlo (MC) solver** typically employed in an iterative scheme with a Computational Fluid Dynamics code (CFD) like e.g. SOLPS-ITER (B2.5-EIRENE). It can track atomic and molecular (A&M) neutrals and ions kinetically, however, ions are mostly handled on the CFD (EDGE2D, EMC3, SOLEDG3X, etc.) side. EIRENE provides in return the momentum, energy and particle sources. A number of such CFD-EIRENE code packages are employed by the fusion community. An essential part of the NGM are the collisional-radiative models (CRMs) for A&M processes involving main-plasma species and impurities. This includes ionization-dissociation-recombination and elastic processes.

EIRENE-NGM is indispensable for both understanding and predicting:

- *the fuel and impurity transport in the edge and divertor (also louvre) areas of fusion devices.*
- *the impurity penetration towards the core*
- *plasma exhaust and plasma-surface interaction (PSI) issues largely determining the duty cycle of ITER and DEMO.*
- *the interplay of transport and A&M processes is the key for understanding of the detachment*



PLOUTOS (web-based A&M data pre-processing and analysis tool)

- **to import/export data (JSON, tabular, etc.)**
- **to produce input data for EIRENE and for other codes with CRMs**
  - ➔ *load/improve/save the developed configuration (selected reactions and parameters) including starting the standard pre-sets*
- **to check data for consistency and abnormal features**
- **do sensitivity studies:**
  - ➔ *understand A&M side of the problem and identify the most significant processes (among the selected ones)*

EIRENE with PLOUTOS

ModCR (CRM module as library with API)

- **both standalone and internal CRM**
- **internal states as variables in MC species**
- **non-stationary approach for A&M processes**

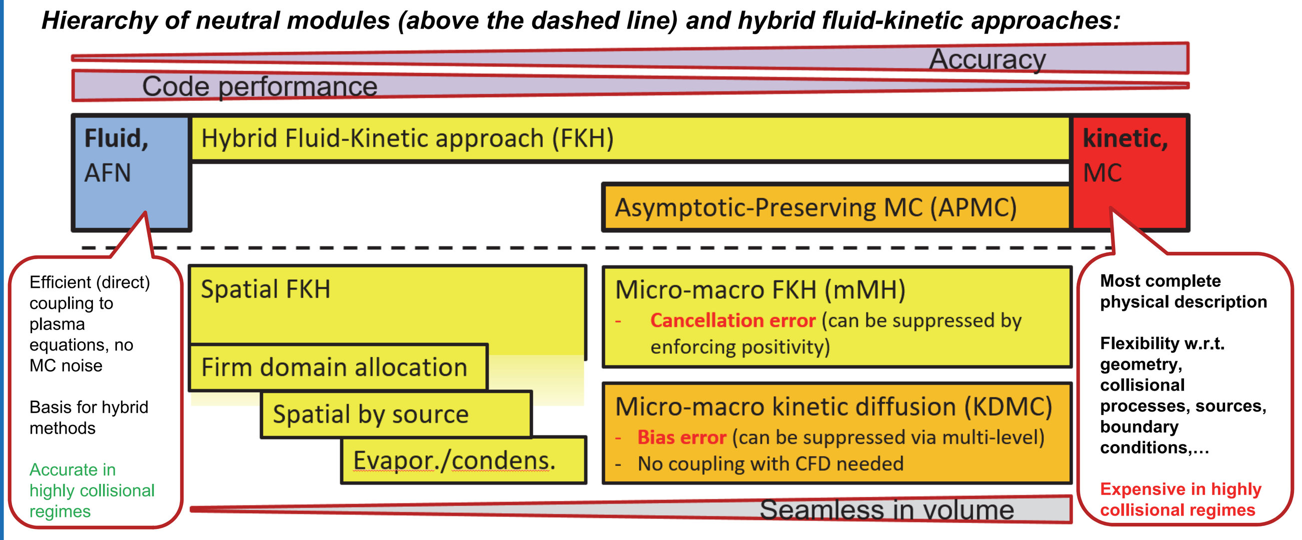
EIRON

EIRON (Toy-model for EIRENE, joint with ACH)

- **testing parallelisation and domain decomposition schemes**
- **optimisation of ML-KDMC and CRM CPU/memory loads**

Fluid-kinetic hybridisation (FKH) approaches relation and basic theory [2]

Hierarchy of neutral modules (above the dashed line) and hybrid fluid-kinetic approaches:



Most developed and tested ***AFN/SpH/mMH branch***:

mMH assumption:

$$f = \sum_i f_i = \sum_i f_i^k + f^f + f^\delta$$

f^f - equivalent to AFN, f_i^k - kinetic terms calculated kinetically by MC approach, f^δ - "kinetic correction", seamless in the entire simulation volume.

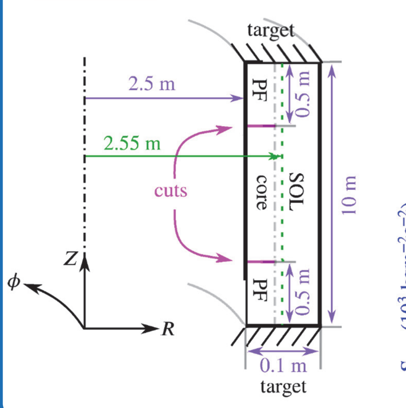
SpH assumption:

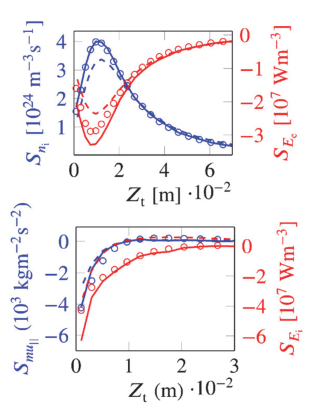
$$\sum_i f_i \approx \sum_i f_i^k + f^f$$

f_i^k assumed negligible in all simulation domains where Knudsen number K_n is sufficiently small, thus AFN is valid (firm allocation) or, alternatively, more flexible approach [21] with evaporation/condensation terms $S_{f\to k}$ and $S_{k\to f}$ is used:

$$\frac{\partial f^k}{\partial t} + v \cdot \nabla f^k = S_c + S_v(f^k) + S_{f\to k} - S_{k\to f}$$

$$\frac{\partial f^f}{\partial t} + v \cdot \nabla f^f = S_v(f^f) - S_{f\to k} + S_{k\to f}$$





An example of FKH simulation (JET-relevant slab, mMH):

- ➔ *hybrid solution approaches the full kinetic one by the accuracy.*
- ➔ *Spead-up factor 5-10 demonstrated*
- ➔ *Similar tests (accuracy and performance) were performed also for other FKH approaches*

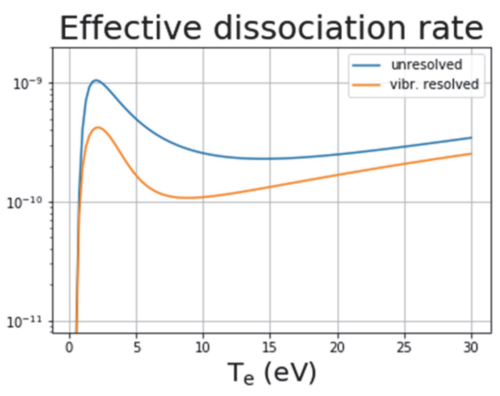
N.Horsten et al., "A hybrid fluid-kinetic neutral model …", **CPP, vol. 60, no. 5-6, p. e201900132, 2020**

NEPTUNE code

➔ ***Asymptotic MC approach – KDMC is under investigation***

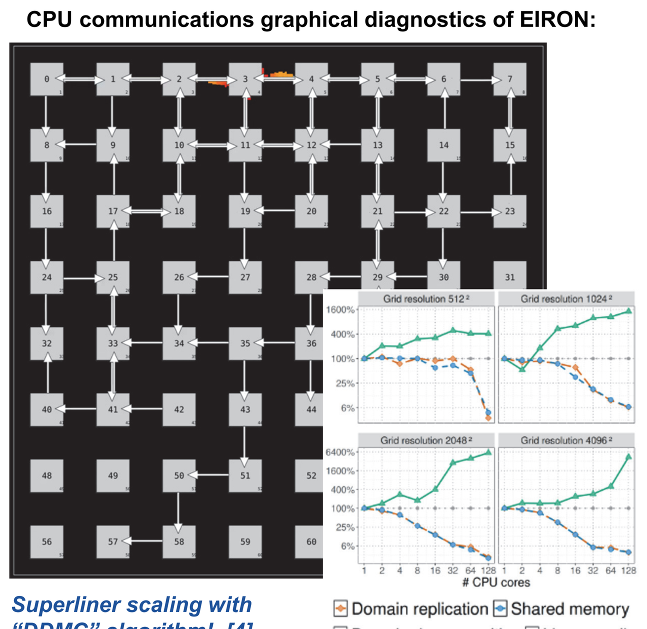
Preceding work in TSVV-5 (2021-2025)

- **EIRENE as** de facto **standard** fully kinetic Monte Carlo **neutral gas module (NGM)** established during TSVV-5 for the EUROfusion and ITER modelling communities.
  - *The **NOV 2024** release of the **milestone version (MsV)** harmonizes multiple versions that were in use in different plasma edge code suites.*
  - *New EIRENE Public License **(EPL)** as accepted by 27 organisations including ITER. It is dual with the open-source CC BY-NC-ND. EIRENE is available at ITER and ACH git repos.*
- **Hierarchy of reduced models (AFN, FKH, KDMC)** is created between AFN and full kinetic solution compromising between accuracy and mathematical rigor.
  - ***FKH** provides essential performance improvement for high-collisional regions critical on ITER/DEMO scale simulations. **Neutral-neutral collisions** were partially implemented.*
  - *The alternative kinetic-diffusive asymptotic Monte-Carlo approach (**KDMC**) is under the investigation and development – new code **NEPTUN** + tests with EIRON.*
  - *This was accompanied with rigorous numerical error analysis. **Algorithmic differentiation (AD)** was implemented for future uncertainty quantification and design studies.*
- **EIRENE-related advanced CRMs** were also largely improved.
  - *Old databases redefined as **PLOUTOS** enabling the realistic practical work on A&M datasets with resolution by vibrational state and isotope.*
  - ***Photon tracing** is now fully available enabling the treatment of opacity and other effects.*
  - *Opacity is proved to be of importance in **validation** runs for existing experiments (e.g. JET). EIRENE performance is also verified with DEMO and ITER PFPO/FPO runs.*
  - *The new module – **ModCR** is concepted to radically improve the treatment of (A&M) processes in EIRENE ridding the main loop of related branching, providing much faster ODE-based solution for internal states. As a standalone option it serves as a reduced model neglecting transport. ModCR is partially completed (data processing and LTE).*
- **EIRENE refactoring, IMASification and parallelisation** has progressed.
  - *Streamlining the main loop, refining the data structure, removing old Fortran constructs like entry points (critical for AD), and improving the **hybrid MPI-OpenMP** parallelization.*
  - *New **JSON input** format provided that fits well to **STYX2.0** coupling and **IMASification**.*
  - ***EIRON,** a new compact code with built-in diagnostics, was developed with ACH-VTT to test parallelization and domain decomposition concepts. It was also used to assess the potential performance improvement of KDMC approach.*



Up to 40% reduction in effective dissociation rate [5] due to transport of vibrational states (for JET) - *both in the full scale EIRENE runs and the stand-alone CRM*

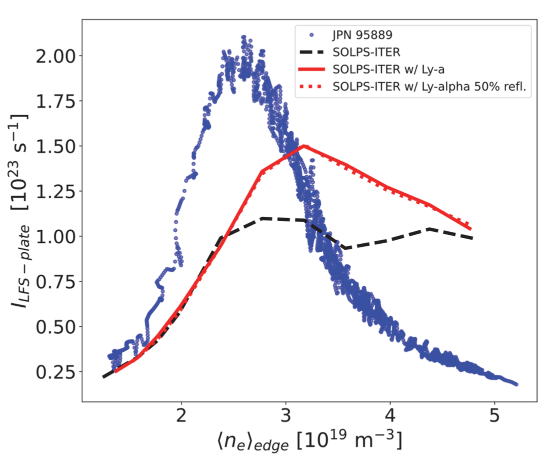
CPU communications graphical diagnostics of EIRON:



Superliner scaling with "DDMC" algorithm! [4]

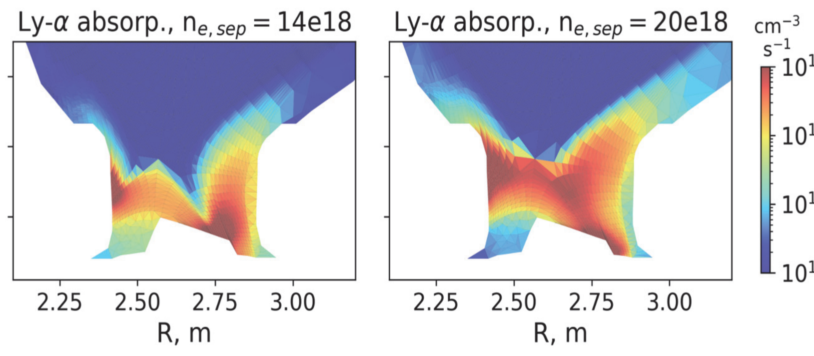
WP2: Development of CRMs - ColRad, ModCR, new datasets in PLOUTOS

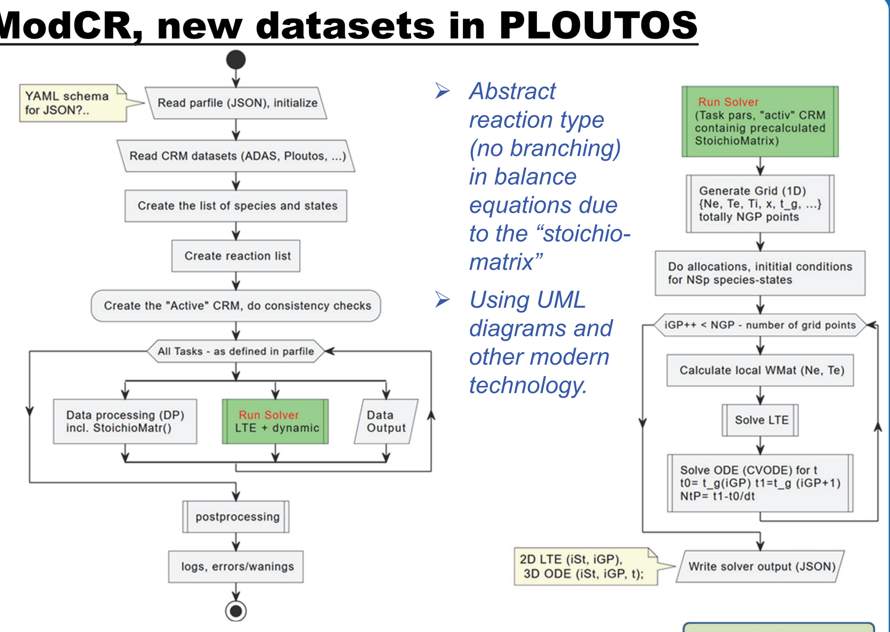
➔ Ly-α and Ly-β opacity, D ionisation, validation [3]



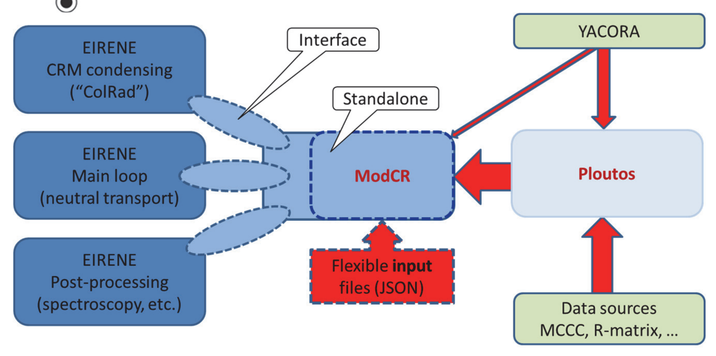
- *Photon absorption adds up to ~20% of total CR ionization rate in detached conditions [6].*
- *Qualitative improvement in D-α Emission validation at JET (L-mode)*
- *Strongly non-local effect impacting detachment*

R. Chandra, et al. PET-20, 2025





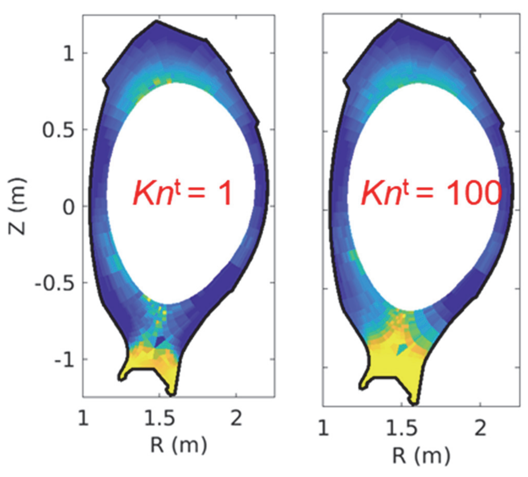
- *Abstract reaction type (no branching) in balance equations due to the "stoichio-matrix"*
- *Using UML diagrams and other modern technology.*

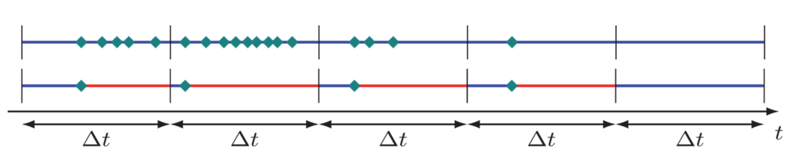


WP1: Continuation of FKH development (AFN with molecules, KDMC)

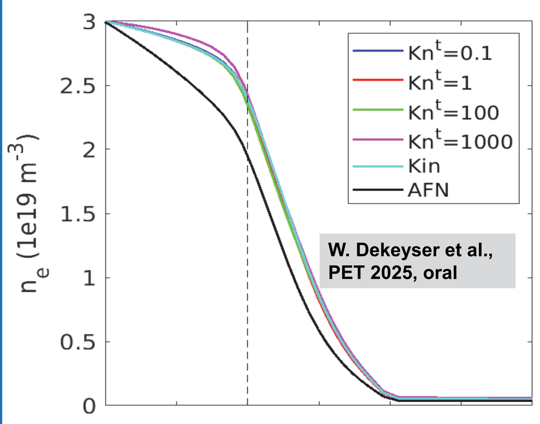
SpH (spatial hybrid.)

~10 times faster than full kinetic





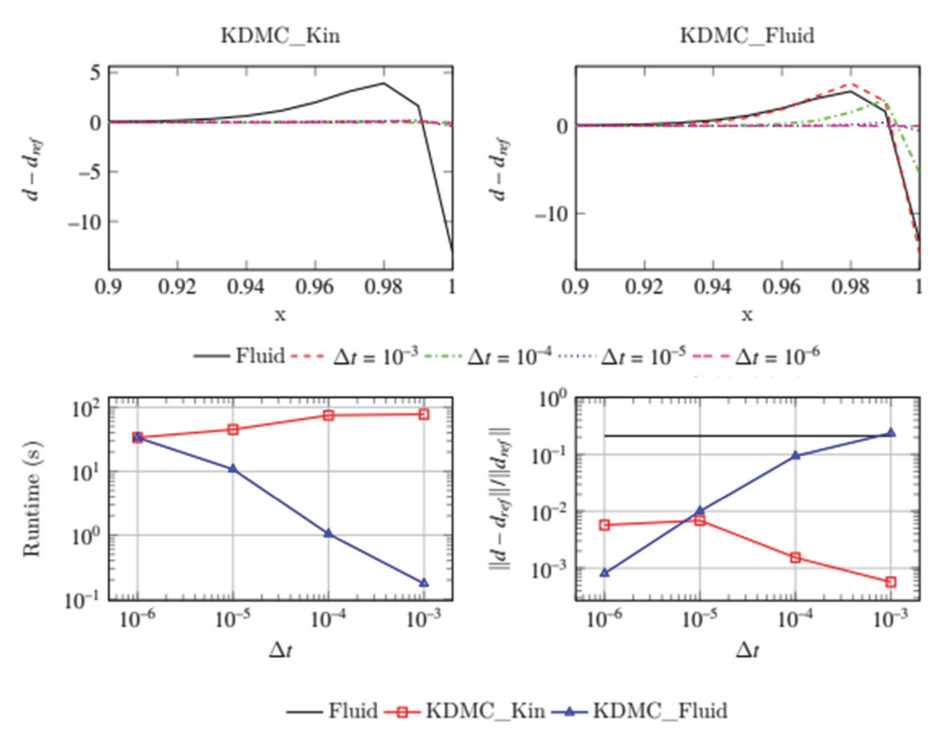
Particle Knudsen number $Kn^{\mathrm{p}} < Kn^{\mathrm{t}}$ *User imposed transition criterion*



W. Dekeyser et al., PET 2025, oral

Kinetic effects corrected by **SpH**:

- *Coupling to void regions beyond plasma grid*
- *Coupling to molecules and impurity neutrals*
- *Kinetic effects in low-collisional regions*



Standard derivation of KDMC close to the boundary (former required full kinetic treatment of relevant species) based on correct distribution taking the boundary condition is provided ➔ **KDMC algorithm is ready for upscaling**

Directions for development in 2026-2027

1. **Refining the AFN model (FKH basis) towards molecules, deriving consistent transport coefficients and boundary conditions.** (WP1)
   a. The combination of atoms and molecules in the fluid models will greatly enhance their reliability, and offer an accurate, noise-free model for simulations at ITER / DEMO scale and implementation in TSVV-B/C codes.
   b. While a fluid model for molecules sacrifices some accuracy in terms of physics, it is expected to greatly reduce computational cost. Moreover, it is expected to alleviate numerical issues related to particle balance in mixed-species processes (e.g. isotope effects in CX collisions and molecular composition), which currently present a bottleneck for, e.g., D-T simulations.
   c. Integration of these extended fluid models in the SpH approach will ensure a correct treatment of kinetic effects in regions and regimes of low collisionality.
2. **Improved Kinetic Diffusion Monte-Carlo (KDMC)** (WP1)
   a. KDMC implementation with the following features: complex geometries through the use of a 3D mesh, accurate boundary conditions by connecting with the TRIM database (both for the kinetic and the fluid boundary conditions).
   b. Full support for heterogeneous plasma backgrounds with physically relevant parameters.
   c. A module that translates EIRENE input to allow users to interface with our code seamlessly.
   d. We note that this implementation will still be based on an atom-only model and will therefore miss the important molecular effects mentioned above. Nonetheless, these models will capture important kinetic effects in non-HCR where pure fluid models are less accurate. Code NEPTUNE is the closest to achieving these goals. Also, EIRON can be used for various tests.
3. **Continuation with the refinement of CRMs** (internal routines like ColRad, external tools Ploutos and the new ModCR module): (WP2)
   a. Adding new datasets recently available from data producers (more species, better accuracy and resolution incl. **vibrational and rotational states** in molecules, bundling and quasi-metastable schemes in atoms; test also **non-stationary approach** in CRMs.
   b. Improving the models e.g. providing the **reflections** in photon tracing, or further investigation of **CXN** parameter distributions.
   c. Prepare **validated datasets** for particular fusion-relevant tasks e.g. characterisation of detachment degree by spectroscopy. Systematic treatment of **D, H, T, He and mixed plasmas :** providing validated isotope-resolved data, demonstrating sufficient performance at ITER and DEMO scales as well as capturing of main physical effects including time-dependent runs.
   d. FAIR data policy (https://www.go-fair.org/) for the A&M and surface (PSI) data – motivated by the IAEA.
4. **Further refactoring of EIRENE-NGM** (**performance** at ITER and DEMO scales) (WP0)
   a. Improving **parallelisation and domain decomposition schemes** utilizing **EIRON** (toy-model) tests and new modular structure.
   b. Providing **code interfaces** with the codes from other TSVVs based on STYX2.0 (e.g. improving treatment of turbulence and PSI effects). Relating the finesse of EIRENE mesh with the one needed for turbulence (both theory and algorithms are needed).
   c. Continuation with the deeper IMASification of EIRENE – more cell types and interfaces. Establishing of further reference simulation cases utilizing the SimDB-based data server (provided in FZJ).

References

[1] D. Reiter, M. Baelmans and P. Börner, *"The EIRENE and B2-EIRENE Codes"*, **Fusion Science and Technology, no. 47:2, pp. 172-186, 2005.**
[2] D.V.Borodin et al., *"Fluid, kinetic and hybrid approaches for neutral and trace ion edge transport modelling in fusion devices"*, **2022 Nucl. Fusion 62 086051**
[3] N. Horsten et al., " Validation of SOLPS-ITER and EDGE2D-EIRENE simulations for H, D, and T JET ITER-like wall low-confinement mode plasmas", ***NME*, 42 (2025) 101842.**
[4] O. Lappi et al.., "Scalable Domain-decomposed Monte Carlo Neutral Transport for Nuclear Fusion", in press, **https://doi.org/10.48550/arXiv.2511.04489**
[5] F. Cianfrani, D.V. Borodin & B. Küppers, *"Data processing and visualization tool for atomic and molecular data for collisional radiative models"*, **Eur. Phys. J. D 77, 139 (2023).**
[6] R. Chandra et al., *"Lyman line opacities in tokamak divertor plasmas under high-recycling and detached conditions"*, **NME (2024), doi: https://doi.org/10.1016/j.nme.2024.101794**
[7] J. Gonzalez et al., "Coupled simulations with SOLPS-ITER and B2.5-Eunomia for detachment experiments in Magnum-PSI", **2023 Plasma Phys. Control. Fusion 65 045009**

Acknowledgement

The EIRENE-NGM package maintained by the FZJ associated developer (AD) community 'JuelichOrigin' is employed. The use and development is licensed under the EPL (see www.eirene.de/EPL) including the related code, data and tools [1, 2].

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