FLUID, KINETIC AND HYBRID APPROACHES FOR EDGE TRANSPORT MODELLING IN FUSION DEVICES

An overview of the efforts to improve the performance of the key simulation tool for the neutral species in the edge of the fusion devices

D.V. BORODIN, F. SCHLUCK, S. WIESEN, D. HARTING, P.BÖRNER, S.BREZINSEK
Forschungszentrum Jülich, Institut für Energie- und Klimaforschung – Plasmaphysik, Partner of the Trilateral Euregio Cluster, 52425 Jülich, Germany

W. DEKEYSER, S. CARLI, M. BLOMMAERT, W. VAN UYTVEN, M. BAELMANS,
KU Leuven, Department of Mechanical Engineering, Celestijnenlaan 300, 3001 Leuven, Belgium

B. MORTIER, G. SAMAEY
KU Leuven, Department of Computer Science, Celestijnenlaan 200A, 3001 Leuven, Belgium

Y. MARANDET, P. GENESIO
Aix-Marseille Univ., CNRS, PIIM, F-13013 Marseille, France

H. BUFFERAND
CEA, IRFM, F-13108 Saint-Paul-lez-Durance, France

E. WESTERHOF, J. GONZALEZ
DIFFER - Dutch Institute for Fundamental Energy Research, Partner in the Trilateral Euregio Cluster, De Zaale 20, 5612 AJ Eindhoven, the Netherlands

M. GROTH, A. HOLM, N. HORSTEN
Department of Applied Physics, Aalto University, Espoo, Finland

H.J. LEGGATE
National Centre for Plasma Science and Technology, Dublin City University, Glasnevin, Dublin 9, Ireland

TH/P2-1

Contact:
D.Borodin@fz-juelich.de

Introduction

Neutral gas physics and neutral interactions with the plasma are key aspects of edge plasma and divertor physics in a fusion reactor including the detachment phenomenon often seen as key to dealing with the power exhaust challenges. A full physics description of the neutral gas dynamics requires a 6D kinetic approach, potentially time dependent, where the details of the wall geometry play a substantial role, to the extent that, e.g., the subdivertor region has to be included. The Monte Carlo (MC) approach used for about 30 years in EIRENE [1], is well suited to solve these types of complex problems. Indeed, the MC approach allows simulating the 6D kinetic equation without having to store the velocity distribution on a 6D grid, at the cost of introducing statistical noise. MC also provides very good flexibility in terms of geometry and atomic and molecular (A&M) processes. However, it becomes computationally extremely demanding in high-collisional regions (HCR) as anticipated in ITER and DEMO. Parallelization on particles helps reducing the simulation wall clock time, but to provide speed-up in situations where single trajectories potentially involve a very large number of A&M events, it is important to derive a hierarchy of models in terms of accuracy and to clearly identify for what type of physics issues they provide reliable answers. It was demonstrated that advanced fluid neutral (AFN) models are very accurate in HCRs, and at least an order of magnitude faster than fully kinetic simulations. Based on these fluid models, three hybrid fluid-kinetic approaches are introduced: a spatially hybrid technique (SpH), a micro-Macro hybrid method (mMH), and an asymptotic-preserving MC (APMC) scheme, to combine the efficiency of a fluid model with the accuracy of a kinetic description. In addition, atomic and molecular ions involved in the edge plasma chemistry can also be treated kinetically within the MC solver, opening the way for further hybridisation by enabling kinetic impurity ion transport calculations. This paper aims to give an overview of methods mentioned and suggests the most prospective combinations to be developed.

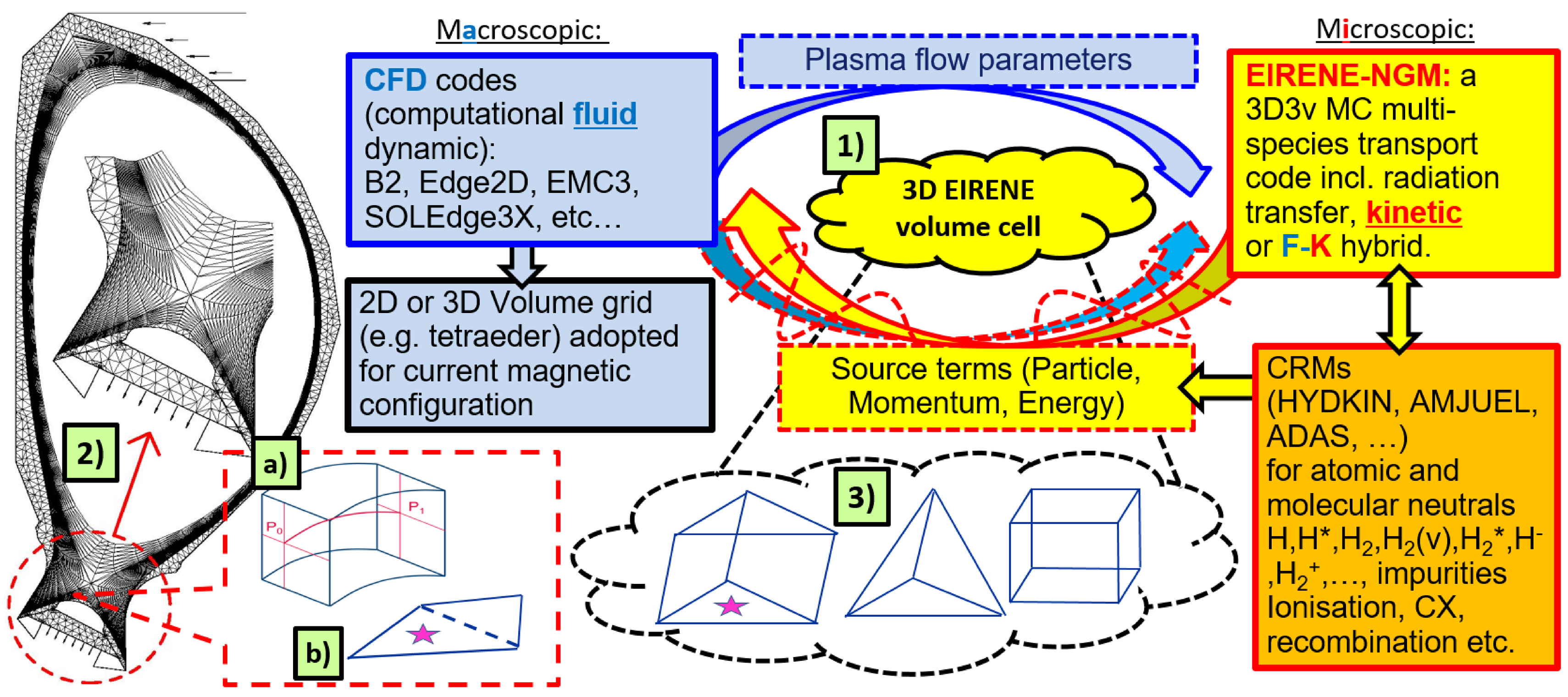


FIG. 1 EIRENE-NGM iterative scheme with the CFD codes; the term neutral gas module (NGM) underlines the role of the code in the coupled packages like SOLPS. 1) The NGM runs simulations for a number of volume cells; 2) The CFD side determines magnetic configuration and runs itself on a grid optimized for it, where the cell shape typically mimics the magnetic field line geometry; this grid may be 3D like in EMC3 a) or 2D, for instance quadrangular plasma cells b) split into triangles in SOLPS-ITER; 3) The EIRENE cells, always 3D, correspond to (or approximate) the CFD cells; for 2D CFD cells an extra dimension is provided (magenta stars mark corresponding triangles in 2D SOLPS and 3D EIRENE cells). EIRENE can run fully kinetic or, alternatively, a fraction of neutrals can be treated as fluid providing higher simulation performance; the corresponding fluid calculations are typically provided by the CFD side. In case of APMC hybridisation no direct coupling with CFD is necessary.

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

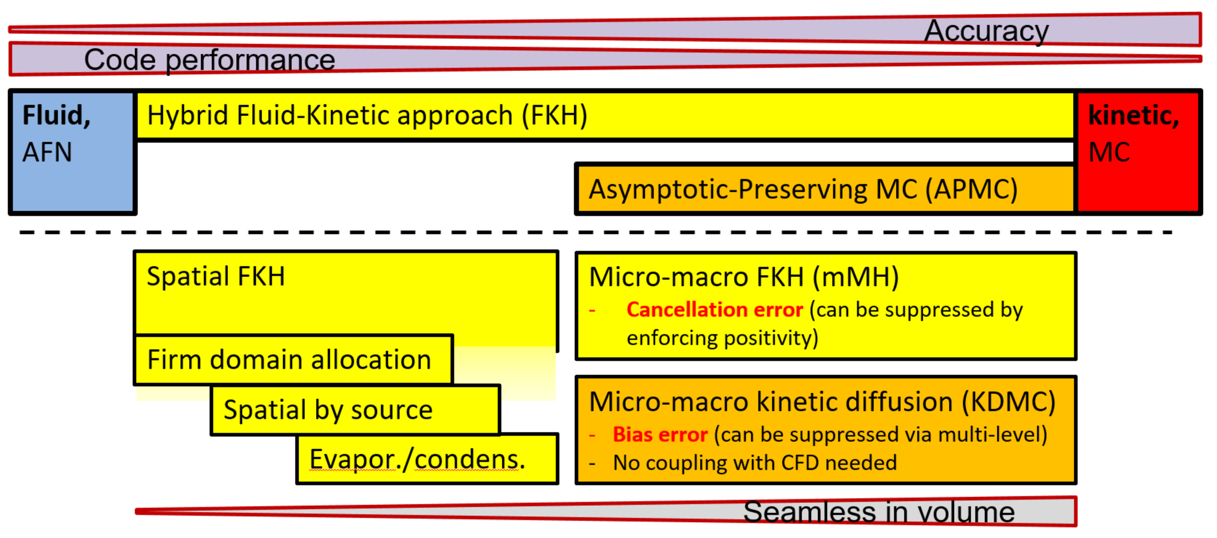


FIG. 4. Hierarchy of neutral modules (above the dashed line) and hybrid fluid-kinetic approaches already implemented in EIRENE (below the dashed line).

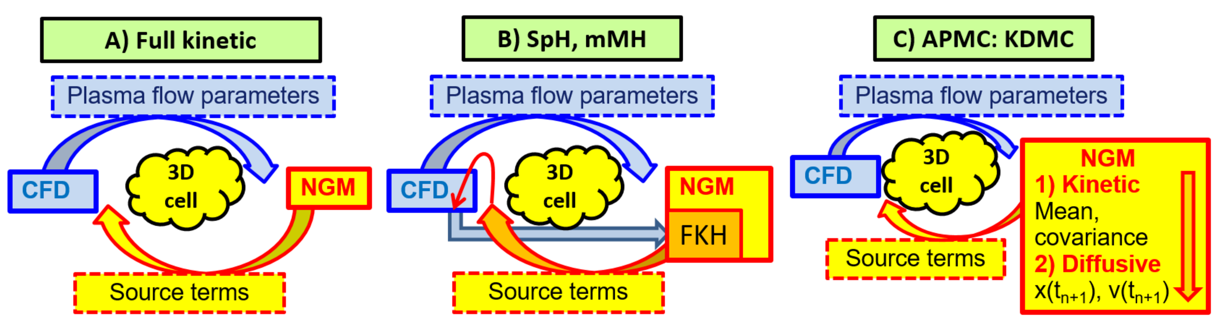


FIG. 5. Central iterative loop (see FIG. 1-1)) in the developed for the EIRENE-NGM FKH approaches.

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:*

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

➔ ***Optional combinations between SpH and mMH methods are subject to ongoing research.***

KDMC (option of APMC) branch:

$$f = \sum_i f_i \approx \sum_i \tilde{f}\left\{\sum_m f_m^{kin}, \sum_l f_l^{diff}\right\}$$

➔ ***Development of an optimal*** $\tilde{f}$ ***estimator is a key element.***

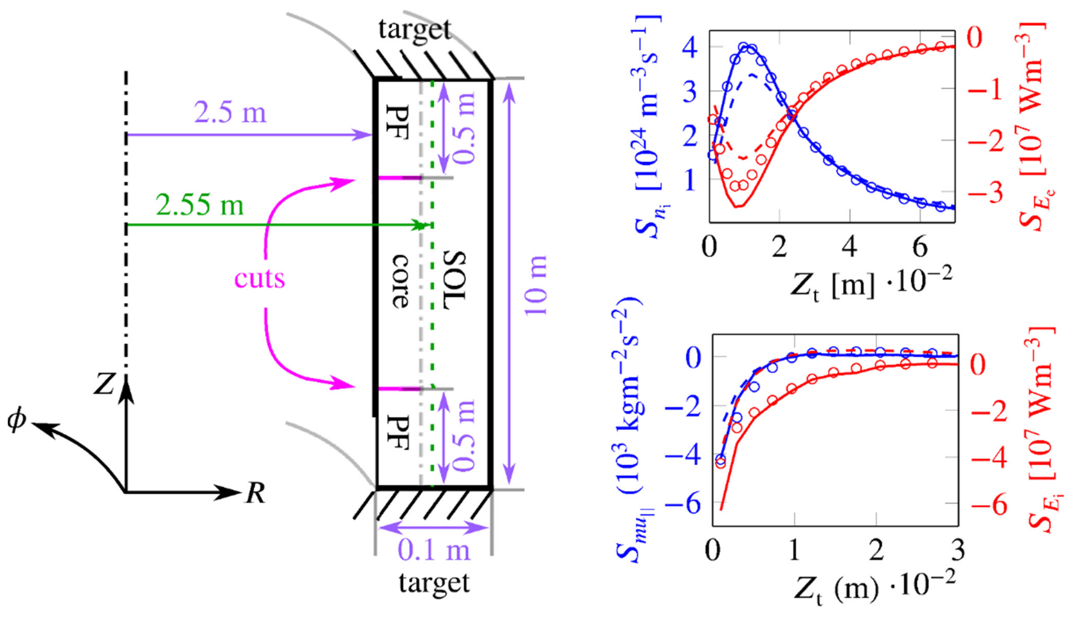
References

[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] H. P. Summers, "The ADAS User Manual, version 2.6," http://www.adas.ac.uk, 2004.
[3] D. Reiter et al., "EIRENE-related data: AMJUEL, HYDKIN, HYDHEL, H2VIBR," http://www.eirene.de/html/a-m_data.html.
[4] U. Fantz, D. Reiter, B. Heger and D. Coster, "Hydrogen molecules in the divertor of ASDEX Upgrade," Journal of Nucl. Materials, vol. 290, pp. 367-373, 2001.
[5] M. Groth et al., "Influence of cross-field drifts and chemical sputtering on simulations of divertor particle and heat loads in ohmic and L-mode plasmas in DIII-D, AUG, and JET using UEDGE," JNM 415.1, pp. S530-S534, 2011.
[6] S. Wiesen et al., "The new SOLPS-ITER code package," Journal of Nucl. Materials, vol. 463, pp. 480-484.
[7] X. Bonnin et al., "Presentation of the New SOLPS-ITER Code Package for Tokamak Plasma Edge Modelling," Plasma and Fusion Research, vol. 11, p. Art.No. 1403102, 2016.
[8] R. Simonini et al., "Models and Numerics in the Multi-Fluid 2-D Edge Plasma Code EDGE2D/U," Contributions to Plasma Physics, Vols. 34 (2-3), pp. 368-373, 1994.
[9] H. Bufferand et al., "Numerical modelling for divertor design of the WEST device with a focus on plasma–wall interactions," Nucl. Fusion, vol. 55, p. 053025, 2015.
[10] H. Frerichs et al., "Stabilization of EMC3-EIRENE for detachment conditions and comparison to SOLPS-ITER," Nucl. Mat. and Energy, vol. 18, p. 62–66, 2019.
[11] Y. Marandet et al., Nucl. Fusion, paper in preparation.
[12] R. A. Pitts et al., "Physics basis for the first ITER tungsten divertor," Nucl. Mat. And Energy, vol. 20, p. 100696, 2019.
[13] H. Bufferand et al., "Progress in edge plasma turbulence modelling – hierarchy of models from 2D transport applications to 3D fluid simulations in realistic tokamak geometry," this conference, 2021.
[14] J. A. Schwartz, E. D. Emdee, R. Goldston and M. Jaworski, "Physics design for a lithium vapor box divertor experiment on magnum PSI," Nucl. Mat. And Energy, vol. 18, pp. 350-355, 2019.
[15] B. Mortier, "Advanced Monte Carlo simulation and estimation for kinetic neutral particles in the plasma edge of fusion reactors," Diss. PhD thesis, KU Leuven, Department of Computer Science, 2020.
[16] N. Horsten, G. Samaey and T. Baelmans, "Development and assessment of 2D fluid neutral models that include atomic databases and a microscopic reflection model," Nucl. Fusion, vol. 57, no. 11, p. 116043, 2017.
[17] J. Fleck Jr and E. Canfield, "A random walk procedure for improving the computational efficiency of the implicit Monte Carlo method for nonlinear radiation transport," Journal of Computational Physics, vol. 54(3), p. 508–523, 1984.
[18] C. Börgers, E. W. Larsen and M. L. Adams, "The asymptotic diffusion limit of a linear discontinuous discretization of a two-dimensional linear transport equation," Journal of Computational Physics, vol. 98(2), p. 285–300, 1990.
[19] A. Crestetto et al., "Kinetic/fluid micro-macro numerical schemes for Vlasov-Poisson-BGK equation using particles," Kinetic& Related Models, vol. 5(4), p. 787, 2012.
[20] M. Blommaert, N. Horsten, P. Boerner and W. Dekeyser, "A spatially hybrid fluid-kinetic neutral model for SOLPS-ITER plasma edge simulations," Nucl. Mat. and Energy, vol. 19, pp. 28-33, 2019.
[21] M. Valentinuzzi et al., "Two-phases hybrid model for neutrals," Nucl. Mat. And Energy, vol. 18, pp. 41-45, 2019.
[22] N. Horsten, G. Samaey and M. Baelmans, "A hybrid fluid-kinetic model for hydrogenic atoms in the plasma edge of tokamaks based on a micro-macro decomposition of the kinetic equation," JOURNAL OF COMPUTATIONAL PHYSICS, vol. 409, p. ARTN 109308, 2020.
[23] B. Mortier, M. Baelmans and G. Samaey, "Kinetic-diffusion asymptotic-preserving Monte Carlo algorithms for plasma edge neutral simulation," Contributions to Plasma Physics, vol. 60, no. 5-6, p. e201900134, 2020.
[24] A. V. Bobylev, "The Chapman-Enskog and Grad methods for solving the Boltzmann equation," Akademia Nauk SSSR Doklady, vol. 262, no. 1, 1982.
[25] R. Schneider et al., "Plasma edge physics with B2-Eirene, Contributions to Plasma Physics 46 (1-2), 2006," Contributions to Plasma Physics, vol. 46, no. (1-2), pp. 3-191, 2006.
[26] M. Blommaert, W. Dekeyser, N. Horsten, P. Boerner and M. Baelmans, "Implementation of a consistent fluid-neutral model in SOLPS-ITER and benchmark with EIRENE," CONTRIBUTIONS TO PLASMA PHYSICS, vol. 58, no. 6-8, pp. 718-724, 2018.
[27] W. Van Uytven, M. Blommaert, W. Dekeyser, N. Horsten and M. Baelmans, "Implementation of a separate fluid-neutral energy equation in SOLPS-ITER and its impact on the validity range of advanced fluid-neutral models," CONTRIBUTIONS TO PLASMA PHYSICS, p. Art.No. ARTN e201900147, 2020.
[28] W. Dekeyser et al., "Implementation of a 9-point stencil in SOLPS-ITER and implications for Alcator C-Mod divertor plasma simulations," Nucl. Mat. and Energy, vol. 18, p. 125–130, 2019.
[29] W. Van Uytven et al., "Comparison of fluid and kinetic models for neutral atoms in realistic plasma edge geometries using SOLPS-ITER," Nucl. Fusion, p. in preparation for submission.
[30] N. Horsten et al., "Application of spatially hybrid fluid–kinetic neutral model on JET L-mode plasmas," Nuclear Materials and Energy, vol. 27, p. 100969, 2021.
[31] C. F. F. Karney, D. P. Stotler and B. J. Braams, "Modeling of neutral plasma in a divertor in the fluid-kinetic transition," vol. 38, no. 1-2, pp. 319-324, 1998.
[32] W. Dekeyser et al, "Plasma edge simulations including realistic wall geometry with SOLPS-ITER," Nucl. Mat. and Energy, p. accepted for publication, 2021.
[33] N. Horsten, W. Dekeyser, M. Blommaert, G. Samaey and M. Baelmans, "A hybrid fluid-kinetic neutral model based on a micro-macro decomposition in the SOLPS-ITER plasma edge code suite," CONTRIBUTIONS TO PLASMA PHYSICS, vol. 60, no. 5-6, p. e201900132, 2020.
[34] B. Mortier, P. Robbe, M. Baelmans and G. Samaey, "Multilevel Asymptotic-Preserving Monte Carlo for Particle Simulations," Submitted to Journal of Computational Physics, 2021.
[35] S. F., "Integration of kinetic ions in a three-dimensional Monte-Carlo neutraltransport code," Contributions to Plasma Physics, vol. 60, p. e201900144, 2020.
[36] M. Baelmans, Blommaert, D. W. M. and T. Van Oevelen, "Achievements and Challenges in Automated Parameter, Shape and Topology Optimization for Divertor Design," Nuclear Fusion, vol. 57, p. Art.No. 036022, 2017.
[37] S. Carli et al., "Sensitivity analysis of plasma edge code parameters through algorithmic differentiation," Nuclear Materials and Energy, vol. 18, pp. 6-11, 2018.
[38] A. Holm, P. Börner, T. D. Rognlien, W. H. W. H. Meyer and M. Groth, "Comparison of a collisional-radiative fluid model of H2 in UEDGE to the kinetic neutral code EIRENE," Nucl. Mat. Energy , vol. doi: https://doi.org/10.1016/j.nme.2021, p. accepted for publication, 2021.
[39] W. Dekeyser et al., "Divertor design through adjoint approaches and efficient code simulation strategies," Contributions to Plasma Physics, vol. 58, pp. 643-651, 2018.

Summary for the gained the fluid-kinetic hybridisation experience

TABLE 1. AN OVERVIEW OF IMPLEMENTED FKH APPROACHES

FKH approach	Main idea and parameter(s)	Advantages	Issues	Development status and performance gain
Advanced fluid neutral models (AFN) [16]	Replace kinetic simulation with a fluid model, tailored to conditions of high CX collisionality	- Large speed-up compared to kinetic simulation (> order of magnitude) - No statistical noise - Tight coupling with plasma equations may improve convergence	- Introduces a modelling error, that may be substantial in low-recycling conditions/regions - Requires a dedicated grid/solver (typically as part of the plasma code)	- Implemented in SOLPS-ITER - Good accuracy for high recycling conditions, incl. ITER, demonstrated [26, 29] - Speed-up factor > 10
Spatial (SpH) – based on source location [30]	Treat neutrals born in high K_n regions as kinetic, and born in low K_n regions as fluid	- Straightforward implementation and coupling to molecules - Clear improvement in accuracy compared to AFN	- (Small) remaining modelling error - Choice of kinetic/fluid source treatment up to user - Sub-optimal speed-up because kinetic trajectories entering HCR not terminated	- Implemented in SOLPS-ITER - Good accuracy for high recycling conditions, incl. ITER, demonstrated - Speed-up factor ~10 demonstrated for JET L-mode discharges, incl. molecules [30]
SpH with evaporation / condensation [21]	Co-existence and interaction of two phases (kinetic and fluid) on the full domain, can be made equivalent to a domain decomposition	More seamless transition, automatic procedure for spatial domains possible	-additional assumptions e.g. CX dominating - more complicated than fixed source treatment, more parameters.	- Implemented in SOLedge2D-EIRENE - potential for speed up demonstrated (30% reduction of EIRENE CPU time in moderately collisional cases) - porting to SOLedge3X and combination with Spatial SpH are in elaboration
micro-Macro (mMH) [22]	Based on exact decomposition of kinetic equation in fluid and kinetic correction parts	Modelling error can be completely removed, at all collisionalities	- Substantial cancellation errors in low collisional /kinetic regions hamper convergence - Requires complete overlap of grids for fluid and kinetic correction neutrals grid (up to the wall)	- Implemented in SOLPS-ITER - Speed-up factor ~5-10 demonstrated in simplified geometries
APMC option: Kinetic diffusion (KDMC) [23] multilevel approach (ML-KDMC [34])	Particles follow a hybridized path that combines advection-diffusion and kinetic steps	-No need to resolve individual collisions -No need for separate fluid/neutral grid - free of cancellation - bias can be suppressed by ML-KDMC	Currently only available for single-species scattering/absorption	The approach is for now just demonstrated on simplified problems, treatment of simulation cases similar to e.g. SOLPS-ITER tasks is in elaboration.



An example of FKH simulation:

➔ *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*

FIG. 2 JET'-relevant by the main parameters slab test case [33] for SOLPS-ITER (including EIRENE-NGM): particle, momentum and energy sources estimated with kinetic (solid lines), fluid (dashed line) and ***mMH*** *(circles) simulations for a flux tube at 2.55 m. One can see that hybrid, in this case mMH, solution approaches the full kinetic one.*

Simulated sightline intensities during the density scan

TABLE 2. ALTERNATIVE WAYS TO INCREASE PERFORMANCE

Approach	Main idea and parameter(s)	Combinability with FKH?	Development status and performance gain
Parallelisation ("brute force" approach)	- Strong scaling allows reducing the wall clock time or improving the MC statistics - Weak scaling allows more detail and larger simulation volume.	Provide additional performance on the remaining kinetic calculation (largest effect expected on APMC where no fluid solver is required for neutrals)	- Good MPI scaling - Decent OpenMP efficiency within 10-20 threads/cores - About 100 times reduction of the memory peak consumption.
Optimised tracking of kinetic processes (selection of critical states, bundled states etc.) [38]	Selection of simulation/estimator procedure based on analysis of variance	- Combination with mMH and SpH straightforward - Combination with APMC (e.g. KDMC) requires new source term estimators	- Results in prototype code, can be transferred to EIRENE
	Improve CRM performance by re-organisation and scalings for e.g. isotopologically resolved hydrogen data	The same reaction rates can be utilized by both the fluid and kinetic parts of FKH codes	- Schemes for CRM construction exist. - Isotopologically resolved hydrogen data is still scarce

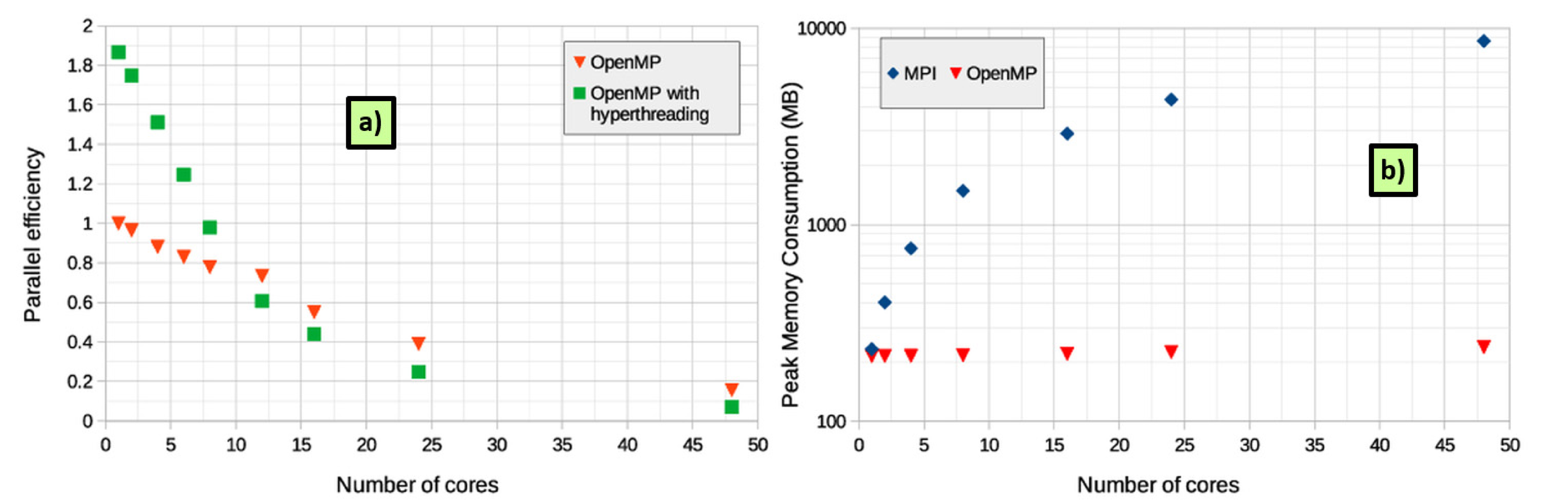


FIG. 3 OpenMP/MPI hybrid parallelisation of EIRENE-NGM demonstrated on the ITER test case. The OpenMP efficiency (left, a) diminishes with the number of cores/threads, however the drop is monotonic and consistent. On a positive side OpenMP provides dramatic reduce of the peak memory consumption (right, b), which is critical for large and detailed simulation cases in particular in a view of the upcoming ITER / DEMO predictive modelling.

Kinetic ion module (KIM) for Atomic and Molecular (A&M) species

- Kinetic Ions followed by **guiding centre** approximation

$$\dot{\vec{R}}_{gc} = \vec{V}_{gc} = v_\parallel \frac{\vec{B}}{B} + \cancel{\frac{\vec{E}\times\vec{B}}{B^2}} + \frac{v_\parallel^2 + v_\perp^2/2}{q_i B/m_i}\frac{\vec{B}\times\vec{\nabla}B}{B^2} + \text{anom. transport}$$

$$\dot{v}_\parallel = \cancel{\frac{q_i}{m_i}\frac{\vec{E}\cdot\vec{B}}{B}} - \frac{v_\perp^2}{2}\frac{\nabla_\parallel B}{B} + \text{coulomb collisions}$$

$$\dot{v}_\perp = \frac{v_\parallel v_\perp}{2}\frac{\nabla_\parallel B}{B} + \text{coulomb collisions}$$

- Currently no electric field in EMC3
- Guiding centre transport by stochastic process

$$\Delta\vec{R}_{gc} = \vec{V}_{gc}\Delta t + \sqrt{D_\perp \Delta t}\,\vec{\zeta}_\perp$$

What is achieved [35]:

➔ *The option is introduced into the EMC3-EIRENE package and applied to a test case relevant for the N_2 seeded ITER scenario (physically meaningful simulations are still in elaboration).*

➔ *First-order drift effects, cross-field diffusion, and magnetic mirror force introduced.*

➔ *Cross-checked on simple model cases against analytical properties of passing and trapped (banana) particle orbits, as well as checking on the introduction of numerical diffusion by our integration scheme.*

➔ *A&M CRMs [2, 3] are made available for KIM (ADAS, AMJUEL, etc.)*

Summary & Conclusions

- **A FKH approach is developed (both SpH and mMH) for the CFD-EIRENE packages [33, 20, 21]. It combines improved computing performance with model accuracy approaching full kinetic simulations.**
- **The alternative perspective APMC approach is also considered [23], including development and first tests of the newly proposed KDMC formulation with a multilevel option [34] aimed to overcome the bias.**
- **In addition, the option to track ions kinetically is improved [35].**
- **The advantages of hybridisation methods are compared based on experience from the first applications to test cases relevant for fusion devices. Currently, the main effort is on**
  a. **basic development of the approaches**
  b. **validation with full-kinetic simulations to determine the gain in computational speedup and optimal parameters**
  c. **impact demonstration of new physics included on, for example, ITER-relevant applications**
  d. **unification of the methods allowing combined mMH and SpH simulations.**

➢ **The hybrid OpenMP-MPI code parallelization and optimisation of the A&M process treatment (improved CRMs) go mostly in parallel adding an additional factor to the improvement of the EIRENE-NGM performance. However, this factor can depend on the final selection of the FKH scheme and overall optimisation of the code.**

EIRENE-NGM-DEVELOPERS

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