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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

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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.

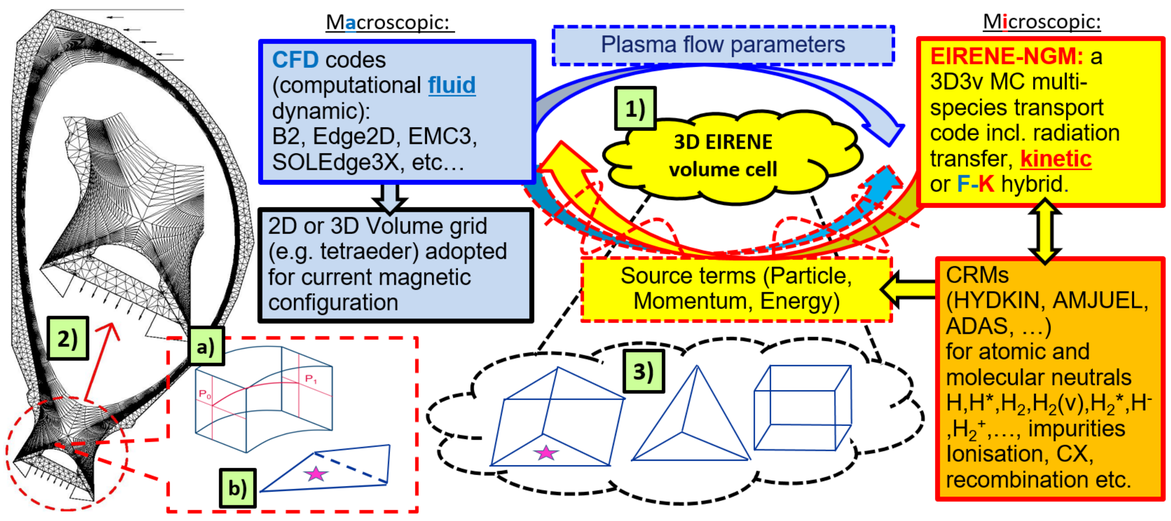


FIG. 1 EIRENE-NGM iterative scheme with the CFD codes; the term neutral gas module (NGM) underlines the role of the code in the coupled packages like SOLPS. 1) The NGM runs simulations for a number of volume cells; 2) The CFD side determines magnetic configuration and runs itself on a grid optimized 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

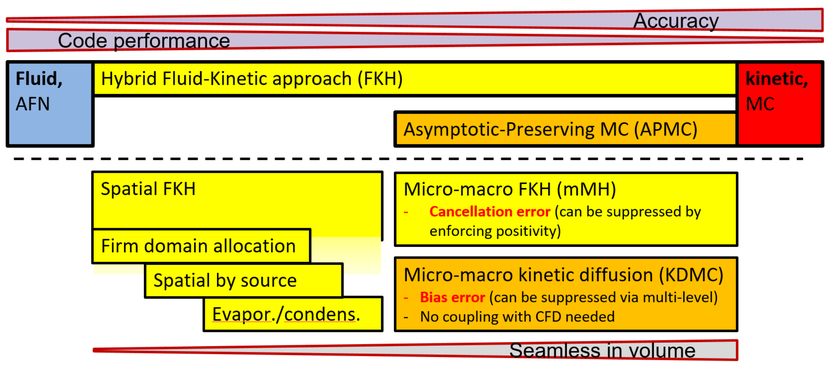


FIG. 4. Hierarchy of neutral modules (above the dashed line) and hybrid fluid-kinetic approaches already implemented in EIRENE (below the dashed line).

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.***

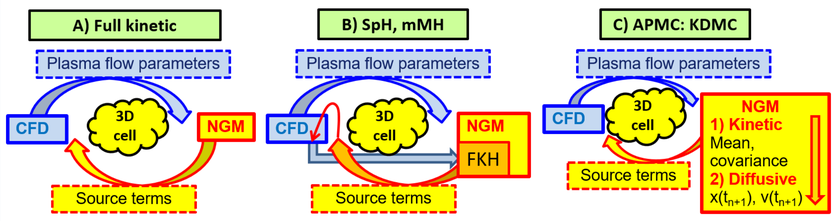
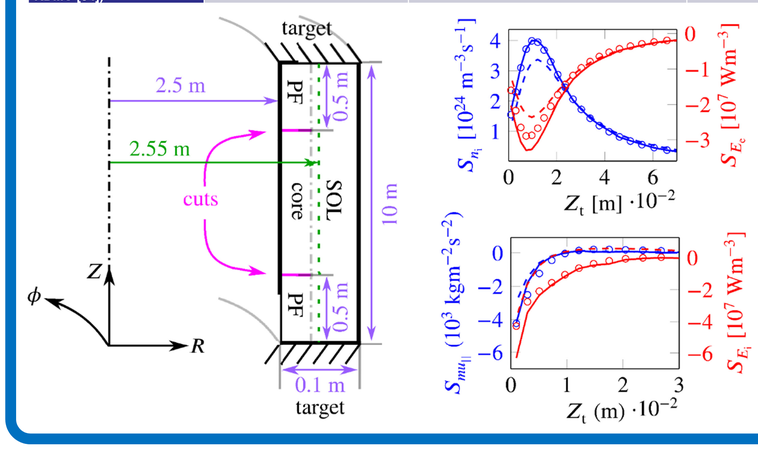


FIG. 5. Central iterative loop (see FIG. 1-1)) in the developed for the EIRENE-NGM FKH approaches.

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.*

Alternative ways to increase the EIRENE-NGM performance

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

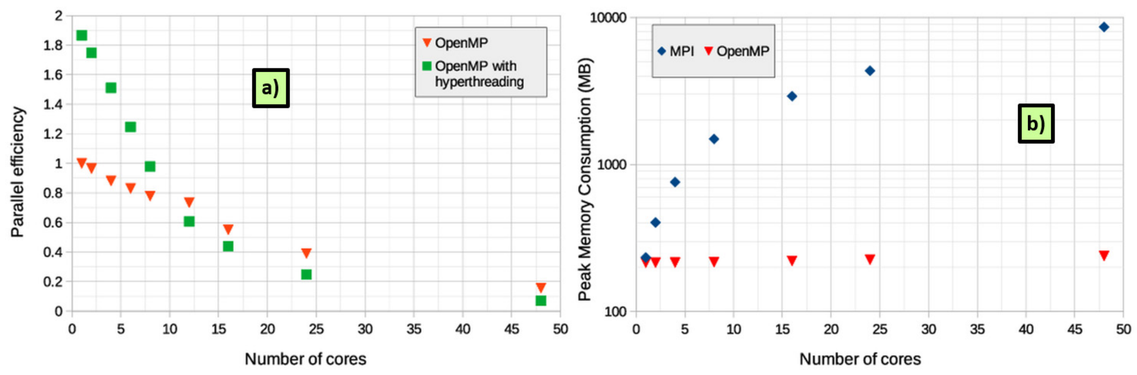


FIG. 3 OpenMP/MPI hybrid parallelisation of EIRENE-NGM demonstrated on the ITER test case. The OpenMP efficiency (left, a) diminishes with the number of cores/threads, however the drop is monotonic and consistent. On a positive side OpenMP provides dramatic reduce of the peak memory consumption (right, 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.**

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EIRENE-NGM-DEVELOPERS

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