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Neptune, KDMC status

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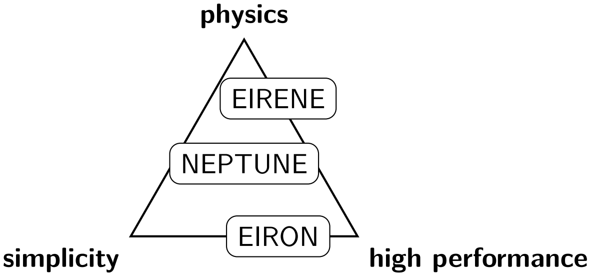
KDMC: very brief recap

- Kinetic Diffusion Monte Carlo (KDMC)
- Three components:
  - Kinetic step: basically standard kinetic solver like EIRENE
  - Diffusive step: brownian motion, an SDE version of AFN. Solved using Monte Carlo, but uses physics from fluid model.
  - Estimation: Information gathered from diffusive step is used as source term in fluid equation. Solved using finite volume method, like the one in SOLPS-ITER.

NEPTUNE: positioning

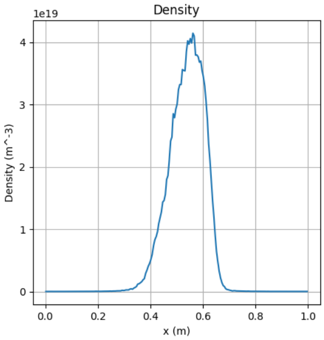
Why NEPTUNE?

- EIRON: not enough physics to really test KDMC
- EIRENE: too complex (for me), KDMC needs to be tested in a simple environment first



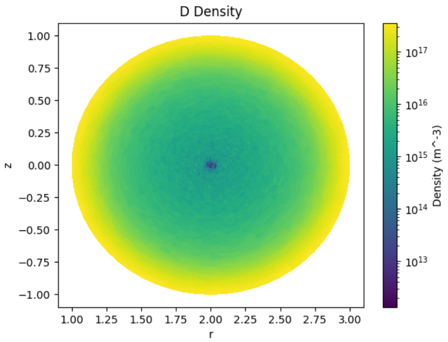
Kinetic step: grid

- 1D, 2D, and 3D structured grids (mostly used for easy testing)



Kinetic step: grid

- 1D, 2D, and 3D structured grids (mostly used for easy testing)
- 2D triangular mesh



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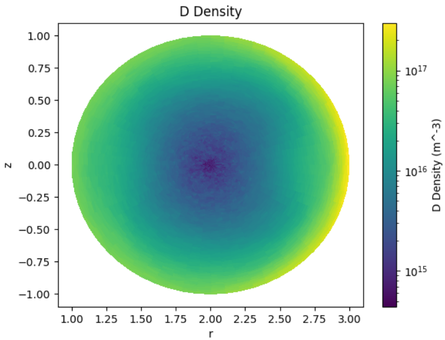
Kinetic step: grid

- 1D, 2D, and 3D structured grids (mostly used for easy testing)
- 2D triangular mesh
- 3D triangular mesh (2D mesh rotated around axis)



Notice that the particles are pushed outwards by centrifugal force

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Kinetic step: collisions

Background collisions:

- Simple collisions ✓
  - Ionisation, charge exchange with multiple backgrounds
  - Rate and new velocity use simple formulas (the ones in Niels' and Vince's paper)
- Planned: AMJUEL (2027)

Boundary collisions:

- Specular with reflection with (partial) absorption ✓
- TRIM: almost done

Sources:

- Volume recombination ✓
- Surface interaction ✓

Diffusive step

Background collisions:

- Simple collisions ✓
  - Ionisation, charge exchange (only one background)
  - Based on rates from kinetic step
- AMJUEL: × will need to use velocity-averaged rates from AFN, not kinetic rates.

Boundary collisions:

- Specular with reflection with (partial) absorption ✓ (required new method development, presented at PET)
- TRIM: × new method should work, will use coefficients from AFN model

Sources ✓ (same as kinetic step)

Estimation

- Very simple advection-diffusion fluid model implemented ✓
- Plan: don't reinvent the wheel, use SOLPS-ITER's fluid solver

Other developments

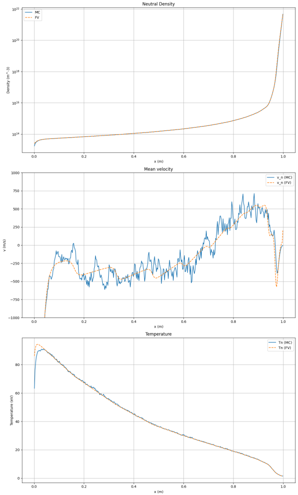
- ARC-MC: modification of KDMC with much better accuracy in intermediate collisionality regimes. ✓
- Improvement of discretisation error in diffusive step: ongoing

Validation

- Results match 1D cases from literature:
  - N. Horsten et al. "Comparison of fluid neutral models for one-dimensional plasma edge modeling with a finite volume solution of the Boltzmann equation"
  - V. Maes et al. "Hilbert expansion based fluid models for kinetic equations describing neutral particles in the plasma edge of a fusion device"
- Validation against 2D cases and EIRENE is needed

1D ITER case

- Simple CX, simple ionisation
- Volume recombination
- Recombination at the wall
- Matches Niels' results



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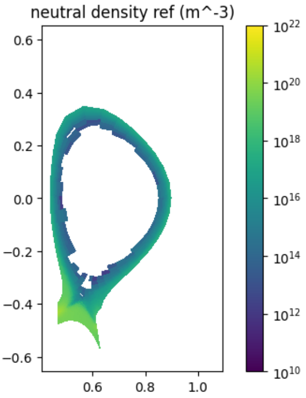
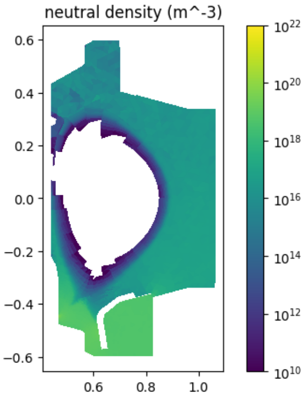
CMOD

Qualitative match, but clear differences

EIRENE



NEPTUNE



IO: Mesh

```
{
    "mesh": {
        "type": "triangle",
        "vertices": [[float, float]], // unit m
        "triangles": [[int, int, int]]
    }
}
```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IO: Collisions

```
{
    "bgk_processes": [
        {
            "rate": [float], // unit 1/s
            "bgk_stddev": [float], // unit m/s
            "bgk_mean_x": [float], // unit m/s
            "bgk_mean_y": [float], // unit m/s
            "bgk_mean_z": [float], // unit m/s
        }
    ]
}
```


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IO: Collisions

```
{
    "ionisation_processes": [
        {
            "rate": [float] // unit 1/s
        }
    ]
}
```

IO: Boundaries

```
{
    "boundary_conditions": [
        {
            "type": "specular"
        },
        {
            "type": "partially_specular",
            "absorption_coefficient": 0.95
        },
    ]
}
```

(a separate list indexes from surface to boundary condition)