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## Particle Simulation of Neoclassical Li<sup>+3</sup> Transport in Realistic Geometry NSTX

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#### **XGC0: Kinetic transport modeling code**

- Full-f Particle-in-cell in 3D magnetic field (RMP, ripple)
- Realistic geometry from geqdsk data (wall and separatrix included)
- 3D (in r-space) + 2D (in v-space) ion and electron Lagrangian dynamics with self-consistent 1D E<sub>r</sub> evolution
- Electrostatic potential  $\Phi$  is assumed to be a flux function
- Logical sheath at diverter plates ( $J_{\perp}$  +  $J_{\parallel}$  =0 out of a flux tube)
- D/H Neutral Monte Carlo particles with a wall recycling coefficient
- Conserving Monte-Carlo Coulomb and neutral collisions (ionization and charge exchange)
- DEGAS2 is built-in (Stotler)
- Multiple ion species with Hirshman collision operator
- Heat flux from core
- Implementation of anomalous transport modeling: random walk and convection. Independent control of the ambipolar particle and the heat transport on each species
- More self-consistent anomalous transport is to be imported from XGC1.
- XGC-RF contains rf operator

#### **Kinetic neoclassical impurity transport simulation**

- Anomalous transport is off  $\rightarrow$  Neoclassical
- Simulation domain:  $\psi_N$ =0.4 to wall in realistic g\_eqdsk geometry (g124439.00497)
- No ripple and RMP
- 5 species:  $D^{+1},\,e^{\scriptscriptstyle -}$  ,  $D^0,\,C^{+6},\,Li^{+3}$
- C<sup>+6</sup> and Li<sup>+3</sup> are born at fixed fraction to  $n_e$ .
- Large initial C density fraction (5% and 10%) and small Li fraction (1/3%)
- Radial transport speeds are calculated from assumed initial profile
- Instead of using DEGAS2, a built-in simplified neutral Monte Carlo model is used for this simulation.
- Self-consistent  $E_r$ - $v_{\parallel}$  with the impurity and edge effects (wall, X-point, neutral, pedestal, etc)

#### Analytic theories are not easy for C and Li impurities

- Large mass ratio and/or high Z approximations are problematic.
- Orbit loss effects (X-loss) on E<sub>r</sub>, rotation and transport are difficult to handle analytically

#### N<sub>e</sub>(r,t) in the simulation



Electron density profiles

#### T<sub>i</sub>(r,t) in the simulation



# At 5% n<sub>c</sub>/n<sub>e</sub>, Li moves inward at much slower speed than C.



#### At $n_c/n_e=10\%$ , Li even moves outward.



#### Impurities affect the $E_r$ -well depth. $E_r$ -well depth at $n_C/n_e$ =10% is weaker than that at 5% (m<sup>-1/2</sup> vs Z<sup>-1</sup> in X-loss)



#### **Physics with conclusion**

- 5 species full-f neoclassical particle simulation in XGC0:
  D<sup>+1</sup>, e<sup>-</sup> , D<sup>0</sup>, C<sup>+6</sup>, Li<sup>+3</sup>
- Realistic NSTX geometry with separatrix and wall, and heat flux from core
- Neoclassical impurity transport is from momentum exchange between the ion species
- E<sub>r</sub> also affects impurity transport (←edge effects)
- For C<sup>+6</sup>, D<sup>+1</sup> is the dominant background species
- For Li<sup>+3</sup>, C<sup>+6</sup> is the dominant background species
- C<sup>+6</sup> moves in while D<sup>+1</sup> moves out.
- Li<sup>+3</sup> moves out relative to  $V_r(C^{+6})$ .
- As C<sup>+6</sup> concentration increases, V<sub>r</sub>(Li<sup>+3</sup>) becomes positive
- More detailed experimental comparison to be performed