- Program Title: Main (local.f95)
- Programming Language: FORTRAN 95
- Subroutines:
    - Initialize – provides formats for all inputs. Reads in values from input file. Begins writing output file (writes initial values to file). Calculates binding energies and migration energies. Sets up mesh? Calculates diffusion coefficients, thermal concentration of vacancies.
    - Prep – sets up DLSODE solver
    - Output – solves for concentration of A atoms, B atoms, C atoms, vacancies, and interstitials. Writes outputs to Unit 6.
    - FEX – computes derivatives using DLSODE solver
    - JEX – required as a dummy variable by the DLSODE solver. Given MITER=2, the analytical Jacobian matrix is generated internally. Subroutine is required for the solver to run, but it does not have any functionality.
- Other files:
    - Unit 5 – perks.in
    - Unit 6 – perks.out
    - Unit 8 – perks.err
- Variables
    - Mesh Definition:
        - R1 – upper bound of region 1 (gb to distance 1 (nm))
        - R2 – upper bound of region 2 (distance 1 to distance 2 (nm))
        - R3 – upper bound of region 3 (distance 2 to distance 3 (nm))

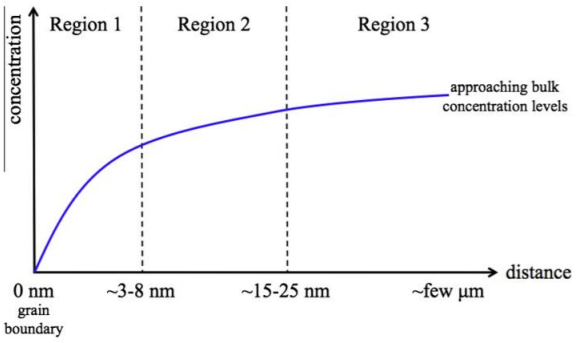

Fig. 1. Schematic of 1-D positional regions in IK model.

        - N1 – number of steps (subdivisions) for mesh in region 1
        - N2 – number of steps (subdivisions) for mesh in region 2
        - N3 – number of steps (subdivisions) for mesh in region 3
    - Tolerances:
        - EPSR – local relative error tolerance for the solution (in DLSODE, RTOL)
        - EPSA – local absolute error tolerance for the solution (in DLSODE, ATOL)
    - Irradiation:
        - DISPRT – displacement rate (dpa/s)
        - ETAV – displacement efficiency for production for freely migrating vacancies

        - ETAI – displacement efficiency for production for freely migrating interstitials
        - DOSE – dose (dpa)
        - TEMPC – irradiation temperature (°C)
    - Concentrations:
        - CONCB – concentration of B atoms
        - CONCC – concentration of C atoms
    - Diffusion:
        - NAT – atom number density
        - LAMBDA – jump distance
        - FAV – jump correlation factor of A atoms to vacancies
        - FBV – jump correlation factor of B atoms to vacancies
        - FCV – jump correlation factor of C atoms to vacancies
        - FI – atom-interstation jump correlation factor
        - WAV – relative vacancy jump frequency for A atoms (normalized to C atoms)
        - WBV – relative vacancy jump frequency for B atoms (normalized to C atoms)
        - WCV – relative vacancy jump frequency for C atoms (normalized to C atoms)
        - WAI – relative interstitial jump frequency for A atoms (normalized to C atoms)
        - WBI – relative interstitial jump frequency for B atoms (normalized to C atoms)
        - WCI – relative interstitial jump frequency for C atoms (normalized to C atoms)
        - NUOV – Debye frequency for vacancies
        - NUOI – Debye frequency for interstitials
    - Cohesive energies:
        - ECOHA – cohesive energy of A atoms (when A=Fe, includes free energy difference between FCC and BCC)
        - ECOHB – cohesive energy of B atoms (when B=Cr, includes free energy difference between FCC and BCC)
        - ECOHC – cohesive energy of C atoms
    - Migration energies:
        - EMIA – migration energy of A atoms by interstitials
        - EMIB – migration energy of B atoms by interstitials
        - EMIC – migration energy of C atoms by interstitials
        - SV – entropy for vacancy formation
        - EMA – migration energy of A atoms by vacancies
        - EMB – migration energy of B atoms by vacancies
        - EMC – migration energy of C atoms by vacancies
    - Formation energies:
        - EFA – vacancy formation energy for A atoms
        - EFB – vacancy formation energy for B atoms
        - EFC – vacancy formation energy for C atoms
        - EFGB – vacancy formation energy for grain boundary atoms

- Ordering energies:
  - EORDAB – ordering energy for A-B atom pairs
  - EORDAC – ordering energy for A-C atom pairs
  - EORDBC – ordering energy for B-C atom pairs
- Material Properties:
  - BIASV – bias factor for vacancies
  - BIASI – bias factor for interstitials
  - Z – recombination volume
  - AL – thermodynamic factor
  - DISL – dislocation density
- Program variables:
  - PSTOP – program stop
  - NOUT – number of output times
  - TOUTPT – time outputs
  - ISTEP – counts iterations
  - IP – an arbitrary number that determines the size of all the arrays