We present a new algorithm that is the key component of our project aiming at a massively parallel off-lattice kinetic Monte Carlo code for heterogeneous systems that will extend the time scale limits of MD to study diffusion at interfaces in concentrated alloys.

**Motivation**
- Point defects - interface interactions
- Segregation and overpopulation of dislocations
- Radiation induced segregation
- Vacancy diffusion makes dislocations to VIMD

**Technological Issues**
- Finding possible events:
  - In crystalline structures, localization of the walkers helps in finding the transition paths.
  - For highly heterogeneous systems, tools like ART (activation-relaxation technique), TAD (temperature accelerated dynamics) or the dimer method may have to be explored.
- Calculate their rates accurately:
  - To achieve the right number for the pre-exponential factor and for the activation barrier will have to be calculated.
- Massive Parallelization:
  - MCMC is tricky to parallelize. Synchronous parallel MCMC.

**Synchronous Parallel kinetic Monte Carlo Algorithm**
- Finite-state MCMC, performs on all defect species and considers property flow.
- Parallelization is tricky because the serial process is the memory cost of each thread.
- For optimum scalability, performance degradation should be subject to the following constraints:
  - First objective: treatment of thermodynamics and displacements in the presence of incoherent interfaces.
  - Second objective: implementation of self-interstitial diffusion.
  - Third objective: Fully parallelization of the code.

**Coupling MD Lammmps – Synchronous parallel kMC**
- Set of possible events.
- Harmonic transition state theory.
- Particle rate: \( \dot{N} = \frac{1}{e^{\left(E_{TS}/kT\right)} + 1} \)
- Diffusive Creep
- Screw dislocation in Cu
- Point defects
- Interface interactions

**Case Studies**
- 001 Coherent Interface Fe-Cr
- Short-Range Order kinetics in Fe-Cr

**Vacancy Accumulation and Jog Formation on an edge dislocation dipole**
- Vacancies (red dots) are inserted at a rate of \( 10^{-12} \text{V/A s} \)

**Vacancy Accumulation and Microstructure Evolution on a 2 degrees Twist Boundary in Fe**
- MC steps = 1
- MC steps = 4901
- MC steps = 10000

**Roadmap**
1. Absorption and recombination of point defects at interfaces
2. Morphological and chemical stability of interfaces
3. Interface-driven mechanical response

**Conclusions and Current Work**
- We have developed a coupled MD-MMC algorithm that allows us to study heterogeneous systems.
- We can reach times far beyond MD capabilities.
- We can take into account long-range fields (e.g., elastic fields).
- Localization of possible events via Voronoi tessellation.
- First nearest neighbors search for heterogeneous structures using Voronoi cell face sharing.
- Improvement of the physics:
  - Calculation of the barriers on the fly
  - Calculation of the prefactors.

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- Interface dislocations seem to be perfect sinks for vacancies. Vacancies accumulate at the dislocation intersections but not at the dislocation intersections.