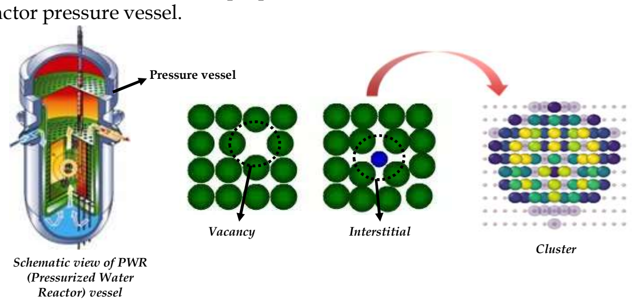
VACANCY ELASTO DIFFUSION AROUND CAVITIES: FIRST PASSAGE ALGORITHMS BASED ON KRYLOV SUBSPACE PROJECTIONS

MODELLING IN NUCLEAR SCIENCE AND ENGINEERING SEMINAR 2020

[1]S. Kaur (savneet.kaur@cea.fr), [1]M. Athènes, [2]J.Creuzé
[1]DES - Service de Recherches de Métallurgie Physique (SRMP), CEA,91191 Gif-sur-Yvette, France
[2]Institut de Chimie Moléculaire et des Matériaux d'Orsay, Université Paris-Saclay, 91405 Orsay, France

Introduction

- Pressurized Water Reactors (PWRs) are subjected to neutron irradiation which introduces many point defects such as vacancies and interstitials.
- These defects migrate, recombine or agglomerate over the time, and forms vacancy clusters or interstitial loops.
- This affects the mechanical properties and embrittle the ferritic steel of the reactor pressure vessel.



Theoretical Formalism

- The early stages of micro-structural evolution are simulated using **Kinetic Monte Carlo (KMC) Simulations** for irradiated nuclear materials.
- Master Equation: $\dot{\boldsymbol{p}}^{T}(t) = -\boldsymbol{p}^{T}(t)\boldsymbol{K}$,where $\boldsymbol{K}$ is Markov matrix of transition rate. KMC method is inefficient when the transition rate matrix describing the evolution of the system exhibits a wide spectrum. System frequently transits between configurations separated by small energy barrier.
- Here, Markov process obeys detailed balance, $\rho_i K_{ij} = \rho_j K_{ji}$ where K_{ij} is transition rate from $i \rightarrow j$ and ρ_i probability to be in state i. This entails K is diagonally similar to symmetric matrix.
- Method to improve KMC: Acceleration techniques based on the theory of **Absorbing Markov Chains** [1]. Absorbing Markov process given as,

$$K^{a} = \begin{pmatrix} -A & A\vec{1} \\ \vec{0}^{T} & 0 \end{pmatrix}$$

- For any probability vector $\pi_t \equiv \pi(t)$, evolving according to master equation [4], the probability of walker in transient and absorbing states is conserved over time and we have, $\pi_t^T = \pi_0^T exp[-K^a t]$.

Methods & Preliminary Results

Matrix Factorization – Allows to sample kinetic paths escaping from the trapping basins [2] (limited to small size trapping basin)

Partial Spectral Decomposition – Excellent approximations of the first passage distributions.

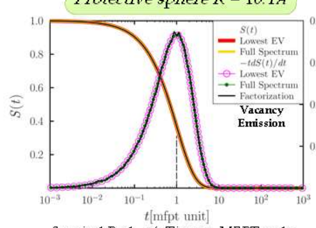
Sparse Eigenvalue Problem

- Symmetric eigenvalue problem: $A^B \varphi_k = \varphi_k \lambda_k$
- Eigenvalue Decomposition with reverse iterations Krylovschur scheme [4]
- Survival probability: $S(t) = \sum_{h=1}^{N} \alpha_h \exp(-\lambda_h t)$,where $\alpha_h = [\pi_0^T \varphi_h][\vec{1}^T \varphi_h]$

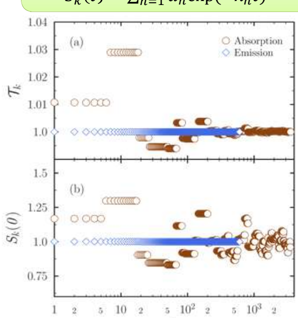
Transient states = 236
Central Cavity R = 4.04Å
Protective sphere R = 10.1Å

Truncation Error, $\mathcal{T}_k = \frac{\sum_{h=1}^{k} \alpha_h/\lambda_h}{\sum_{h=1}^{N} \alpha_h/\lambda_h}$

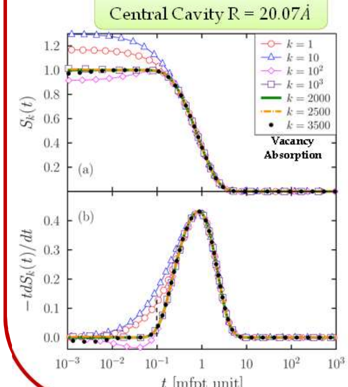
$S_k(t) = \sum_{h=1}^{k} \alpha_h \exp(-\lambda_h t)$



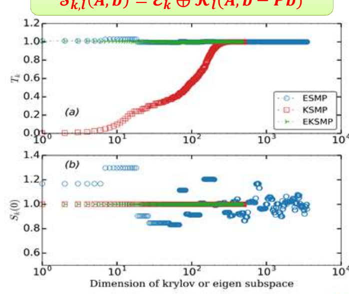
Survival Prob. v/s Time on MFPT scale



Transient states = 34801
Central Cavity R = 20.07Å



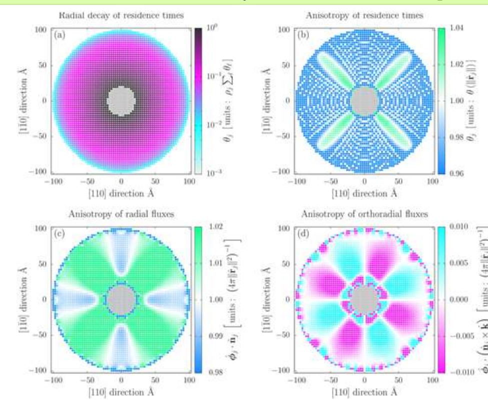
RESTARTED KRYLOV SUBSPACE:
$\mathcal{S}_{k,l}(A,b) = \mathcal{E}_k \oplus \mathcal{K}_l(A, b - Pb)$



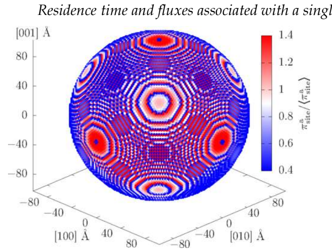
Sparse Linear System

- Linear System solved using Iterative and Direct solvers
- MFPT = Sum of residence times from initial state ($A\tau = \vec{1}$)
- Residence time: $\theta^T A = \pi^T$

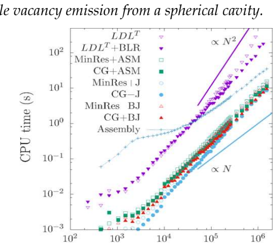
Single vacancy emission from cavity (2243 vacancies in cavity) at T = 600K
N = 259320 Transient states with Cavity R = 20.07Å, Protective sphere R = 101Å



Residence time and fluxes associated with a single vacancy emission from a spherical cavity.



Absorbing Probabilities: Anisotropy on peripheral sites



Comparison between Iterative & Direct Solvers

Summary and Ongoing Work

- ✓ Theory of Absorbing Markov chains and applications to diffusion process.
- ✓ First passage problem simplified by exploiting the property of reversibility.
- ✓ Krylov subspace projection methods for sparse linear system and eigenvalue problems are efficiently implemented [4].
- ✓ First passage distributions and probability fluxes are obtained in realistic problem.
- ✓ Estimation of residence times and fluxes associated with vacancy emission [3].
- ✓ Iterative solver performs better than direct solvers – by a factor of 10-20 [4].
- ✓ Krylov subspace projection (small basis) method to apply a vector on a matrix function is being implemented.

References

[1] An energy basing finding algorithm of Kinetic Monte Carlo acceleration, B.Puchala, M.L.Falk, and K.Garikipati, *J. Chem. Phys.* **132,134104 (2010).**
[2] Path Factorization Approach to Stochastic Simulations, M.Athènes, and V.Bulatov, *Phys. Rev. Lett.* **113, 230601 (2014).**
[3] Effect of saddle point anisotropy of point defects on their absorption by dislocations and cavities, D.Carpentier, T.Jourdan, Y.Le Bouar, M.C.Marinica, *Acta Mater.* **136 323-334 (2017) .**
[4] Elastodiffusion and cluster mobilities using kinetic Monte Carlo simulations: Fast first-passage algorithms for reversible diffusion processes, Manuel Athènes, Savneet Kaur, Gilles Adjanor, Thomas Vanacker, and Thomas Jourdan, *Phys. Rev. Materials* **3, 103802 (2019).**