SciDAC – PSI:
Plasma Surface Interactions Involving He

Brian D. Wirth*,#, on behalf of

In partnership with: FASTMATH, QUEST, SDAV (Scalable Data Management, Analysis, and Visualization), SUPER (Institute for Sustained Performance, Energy, and Resilience)

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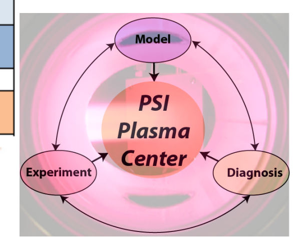

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UMass Amherst · Illinois · UC San Diego · General Atomics DIII-D National Fusion Facility · Pacific Northwest National Laboratory · Argonne National Laboratory · Los Alamos National Laboratory · # Oak Ridge National Laboratory · The University of Tennessee Knoxville

SciDAC Project Web Site: https://collab.mcs.anl.gov/display/PSIscidac/

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*The Challenge of Plasma Surface Interactions**

• Plasma facing components (PFCs) must remove plasma exhaust, which involves unprecedented power and particle fluxes & fluences, while limiting release of impurities to core plasma

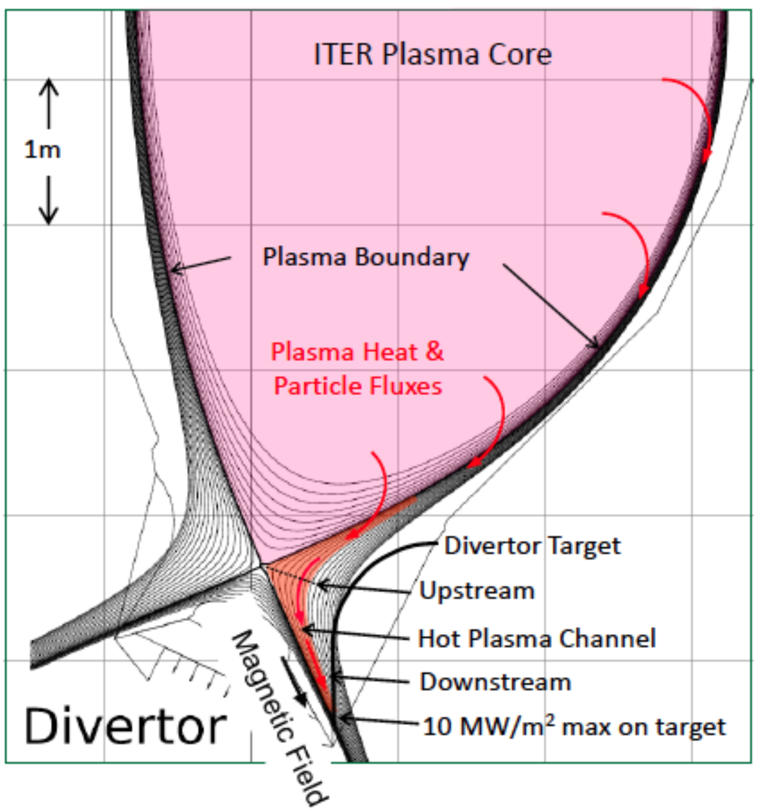
<u>Key Issues</u>
- Erosion lifetime and plasma compatibility
- Tritium inventory
- Thermal transients
- H/He blistering
- Heat removal
- Fabrication technology
- Neutron damage

<u>Leading candidate materials</u>

PFC and Divertor
- Be, W, (C?)

Structural components
- Fe-Cr steels, V-Cr-Ti, SiC

ITER Plasma Material Interface



bulk plasma:
impurity tolerance
W < 2 10^{-5}, reactor < 10^{-4}
Be, C: 10^{-2}

first wall:
modest flux of high energy neutral particles (100s eV),
low energy ions

divertor target:
high heat flux 10 (20) MW/m²
<u>transient heat loads</u>:
e.g. ELMs, disruptions

Additional challenge involves chemistry evolution, as well (erosion, transport, re-deposition)

***Ref: H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany**

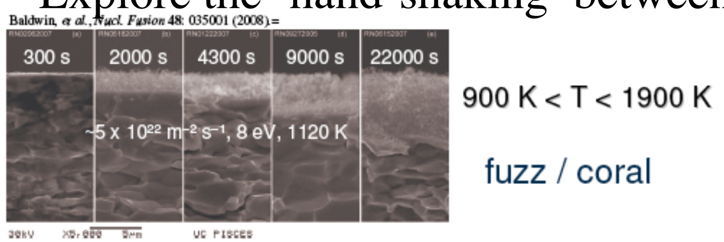
SciDAC – PSI Objectives & Approach

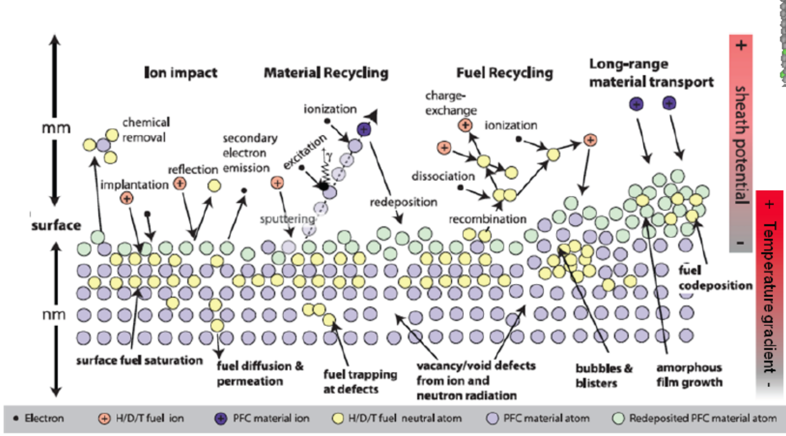
• Develop simulation capability for plasma surface interaction across three coupled spatial regions:

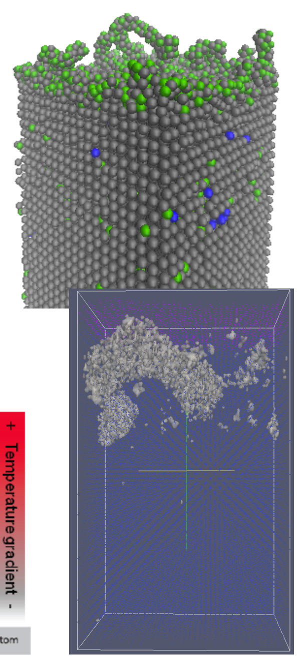
- **Edge/scrape-off-layer region of the plasma (X. Tang, J. Canik)**
- **Near surface material response to plasms exhaust, with neutron damage and influenced/ coupled to plasma sheath (B.Wirth, B. Uberuaga, D. Maroudas)**
- **Structural materials response to intense, 14 MeV-peaked neutron spectrum (R. Kurtz)**
- **Experimental validation interface/database (V. Chan, D. Ruzic)**

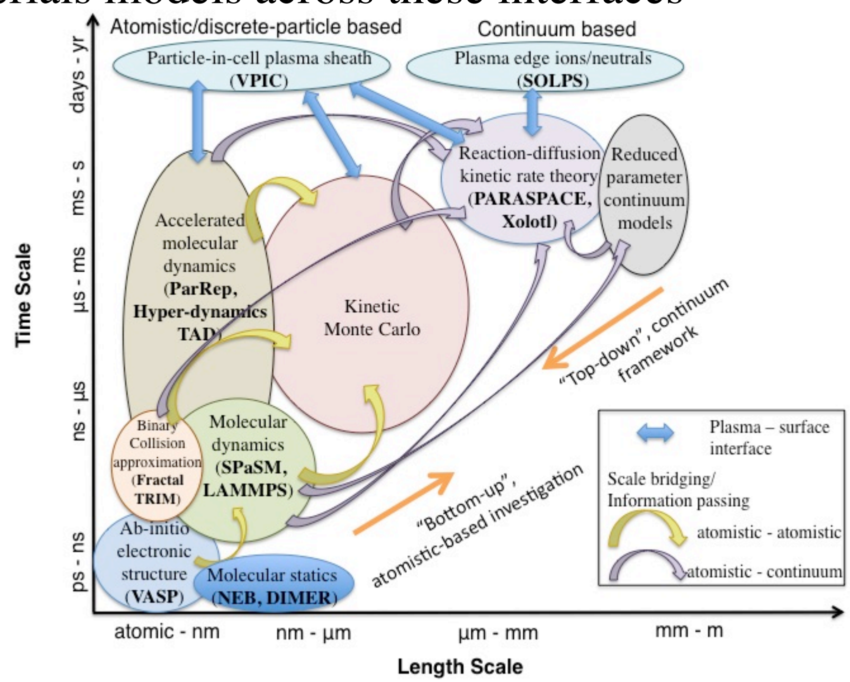
• Simultaneous 'bottom-up' and 'top-down' approach to multiscale modeling that integrates SciDAC institute capability into both particle and continuum based codes, and develops from scratch a new code, Xolotl for PSI

• Explore the 'hand-shaking' between plasma and materials models across these interfaces









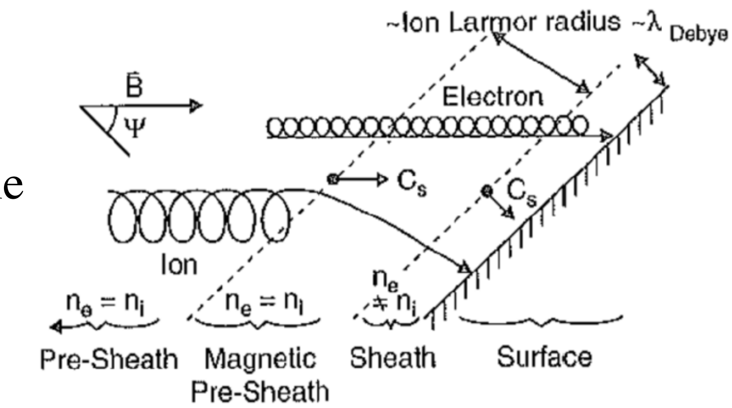
Plasma edge/scrape-off layer: SOLPS

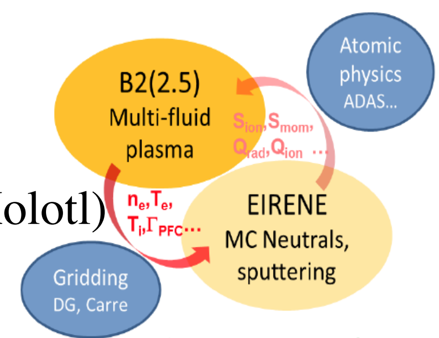
- **Plasma modeling utilizes both particle- and continuum-based approaches**

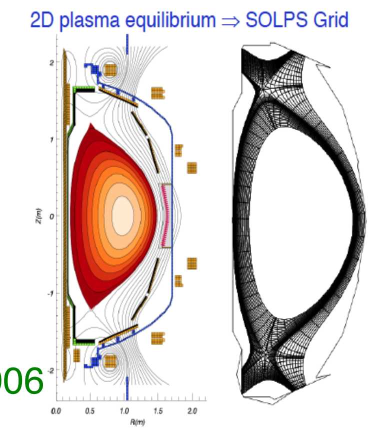
- Near surface sheath region treated with particle-in-cell code (VPIC); kinetic approach needed to caclulate particle trajectories, electric & magnetic fields

- Plasma/neutral transport in pre-sheath edge/scrape-off layer simulated using SOLPS code*

  - 2D transport: radial & poloidal
  - Fluid equations solved for plasma ions
  - Classical transport parallel to magnetic field
  - Neutral transport by Monte Carlo
  - EIRENE simulates PSI (eventually replaced by Xolotl)







* Schneider, CPP 2006

- **Evaluation of SOLPS performance (Roth)**

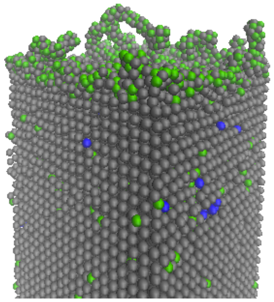
SOLPS performance on KIDS

nThreads	user (s)	system (s)	elapsed (m:s)	CPU (%)	CPU/thread
1	103.45	1.72	02:05.6	83.33	83.33
2	185.56	4.97	01:51.7	170.33	85.17
4	373.19	12.86	01:50.8	348.00	87.00
6	583.76	17.37	01:54.7	523.67	87.28
8	792.94	25.27	02:05.2	653.67	81.71
12	1203.57	44.45	01:58.8	1050.67	87.56

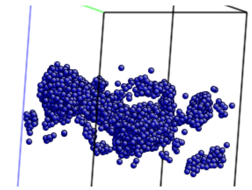
Lots of time spent on i/o, waiting

- Loop at b2news.f:488 25.8%
- b2npmo 18.8%
- b2npht 16.5%
- Loop at b2news.f:355 13.3%

- function loop evaluation: HPC toolkit (http://hpctoolkit.org)



Solid Surface Modeling Roadmap



Low temperature (< ~1000 K) regime of low-energy (~100 eV)
He (later mixed He-H) plasma exposure to tungsten, focused on bubble formation, growth & over-pressurization leading to tungsten surface morphology changes

Key Physics Questions:

- Rate effects (AMD, MD and KMC) versus continuum reaction-diffusion & experiment
- Dilute limit approximations in concentrated He bubble populations
- Biased/drift diffusion (elastic strain field interactions that add drift term to diffusional flux)
- Multiscale integration

Dilute limit (?)

(Additional) collective phenomena
(mixed species, higher T, etc.) →

Diffusion drift aggregation theory

Visualization/ post-processing

Comparison with data – what observables?

Parametric studies

"Integrated bubble evolution modeling" & inter-comparison (bubble dynamics, etc…)

'Individual effects' (e.g., bubble bursting, drift-diffusion)

Continuum models with explicit presence of bubbles that need to be discretized (front-tracking)

Diffuse interface models (e.g., phase field)

Eventual development of model reduction (UQ) to reduce species tracking

Paraspace (initially) - XOLOTL-PSI

Both input (multiscale linking)
& comparisons of predictions

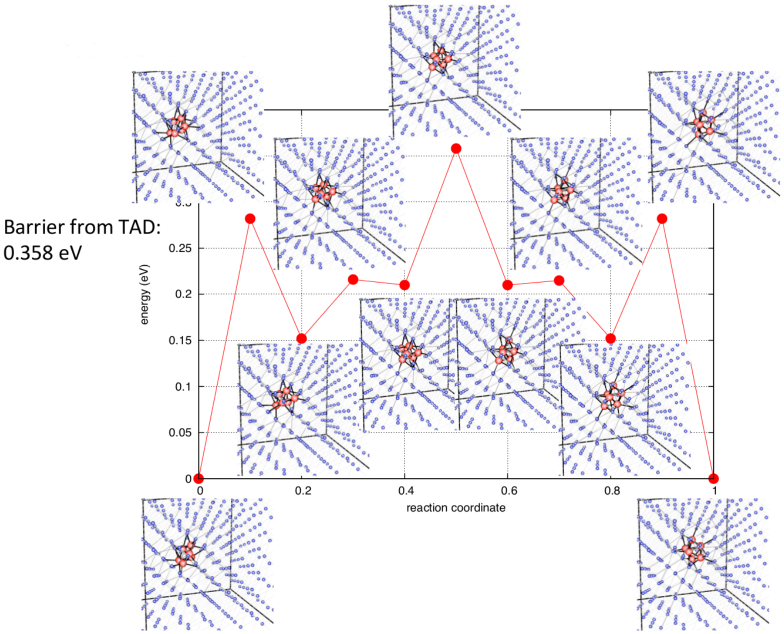
MD/AMD/KMC

Near surface to bulk → matching ←

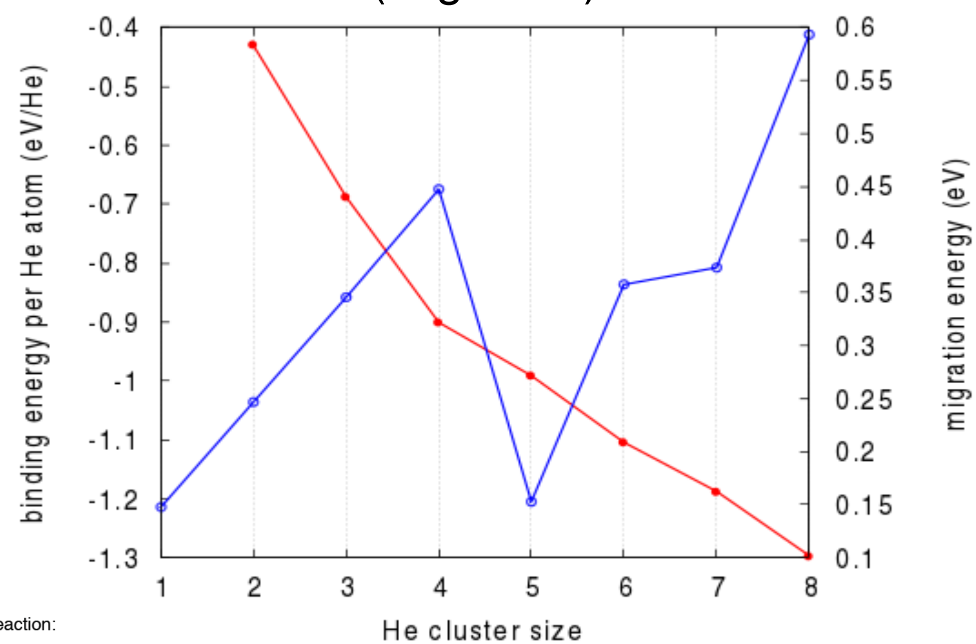
*Thermodynamics & kinetics of small He clusters**

- **Atomistic simulations (AMD, MD, statics) used to identify unit transport/reaction mechanisms**
  - Challenges relate to multitude of pathways with increasing cluster size

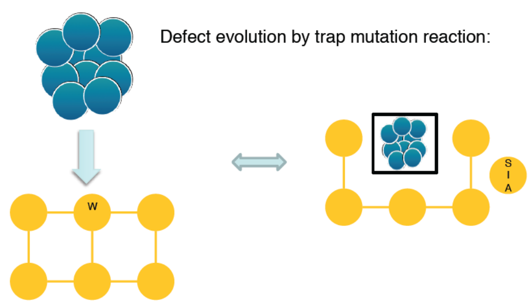
4-He cluster migration:



Thermodynamics (binding) & kinetics (migration):



Larger clusters undergo 'trap' mutation which decreases mobility



Monotonic increase in binding energy,
Complex, size-dependent kinetics

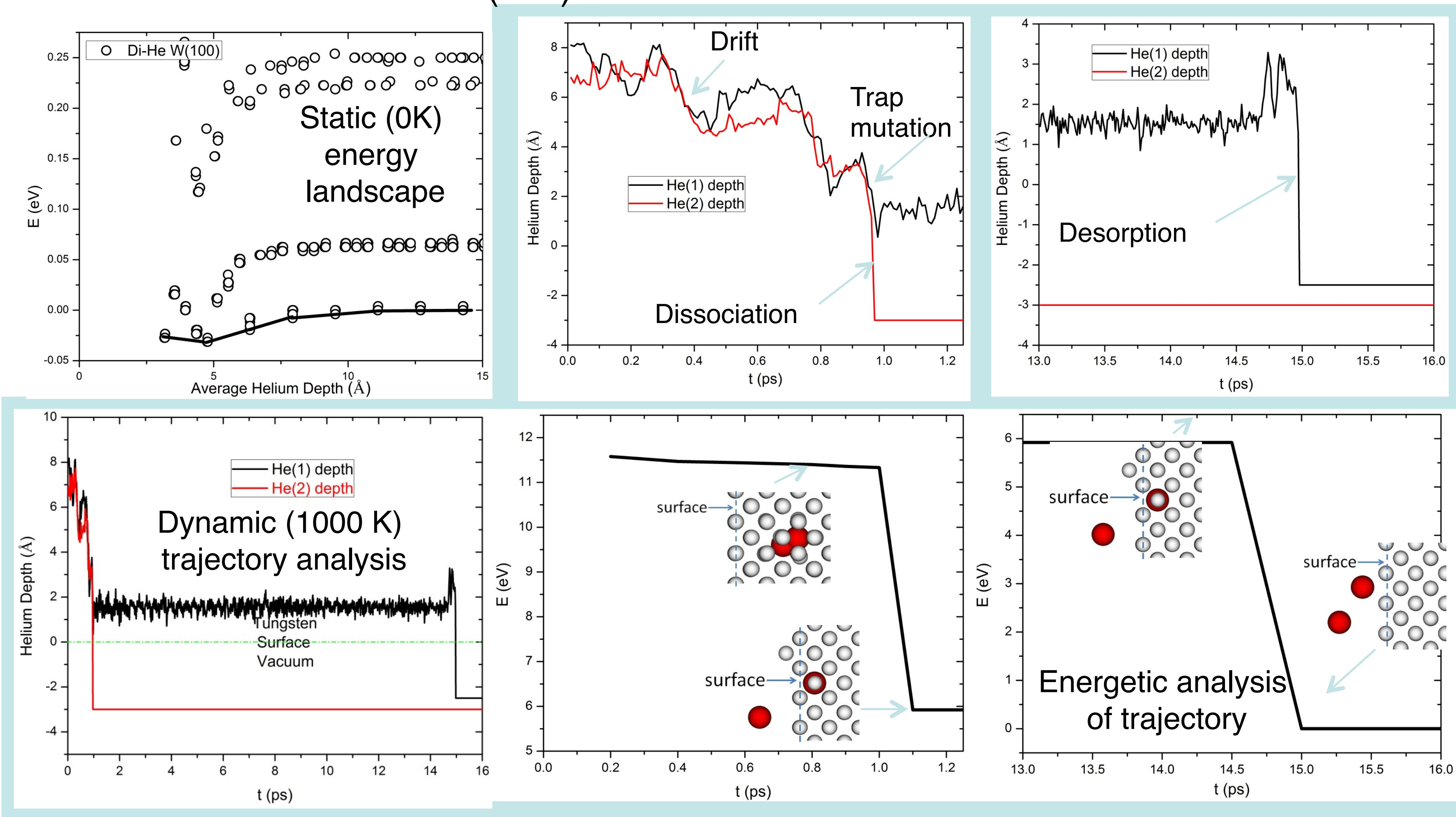
- Ken Roche initiated effort with AMD team to evaluate/improve code performance

* Uberuaga et al., manuscript in preparation

*Surfaces modify behavior of small He clusters**

- **Atomistic simulations identify 'drift diffusion' interaction of He clusters with surfaces/ extended defects, and modification of kinetics by 'trap mutation'**

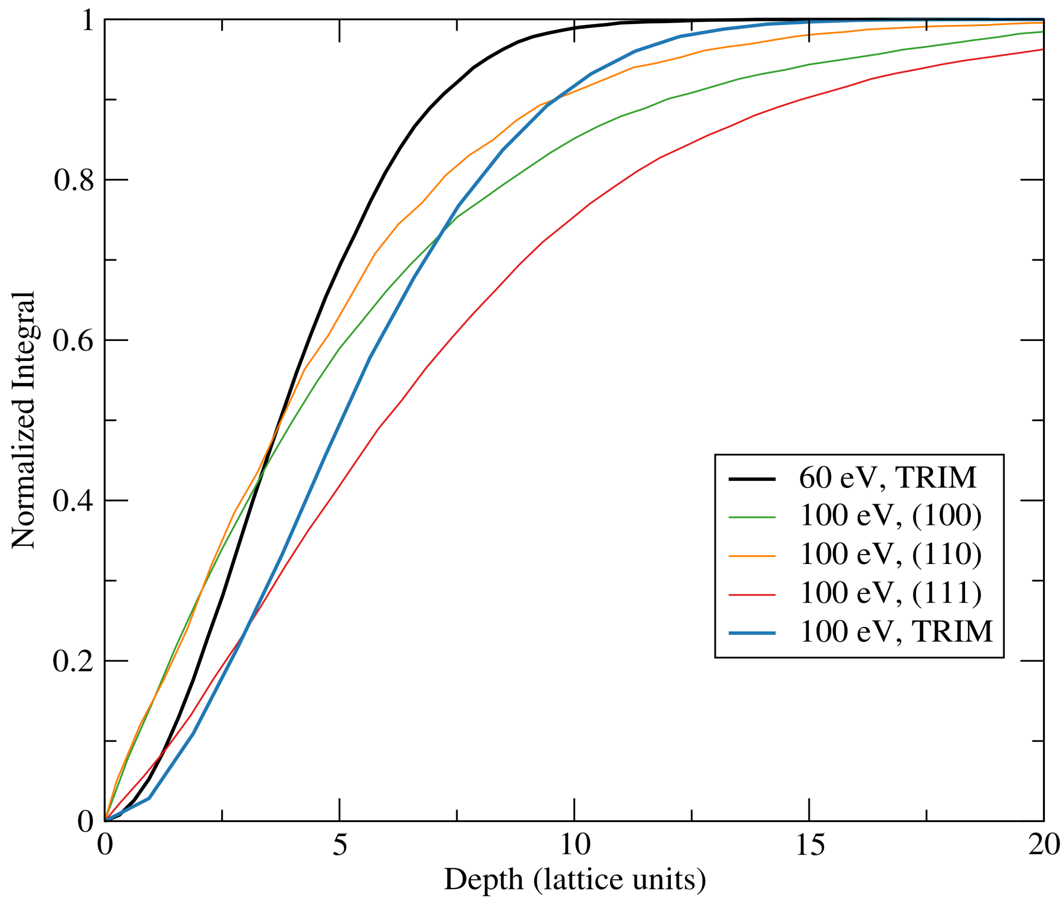
Di-helium interaction with (100) surface



* Hu et al., manuscript in preparation

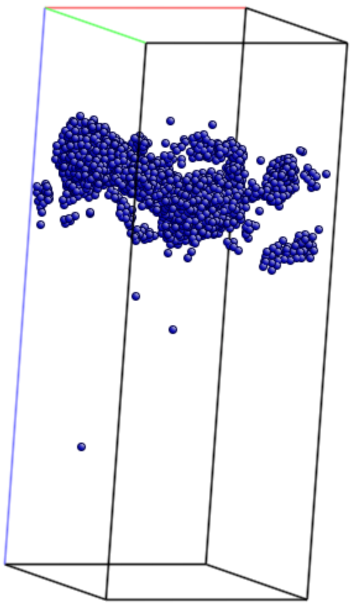
Atomistic investigation of early stage He bubble evolution

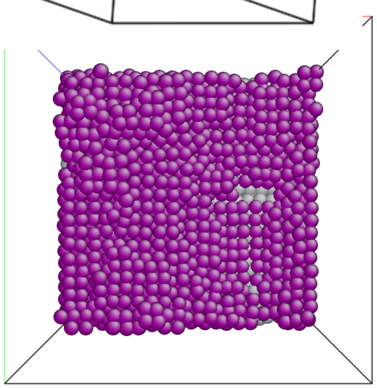
- **Tungsten with (100) or (111) surfaces**
- **Periodic boundaries in the x, y directions and Free Surface in z**
- **Single crystals versus specimens containing Σ3 or Σ5 grain boundaries (intersect surfacee)**
- **Every 10 ps a He atom is added according (implanted) based on He depth distribution of 60/100eV He flux**
- **Temperatures between 500-2000K**
- **10 simulations for each temperature**
- **→ Quantify He cluster/bubble size distributions as a function of time/fluence**

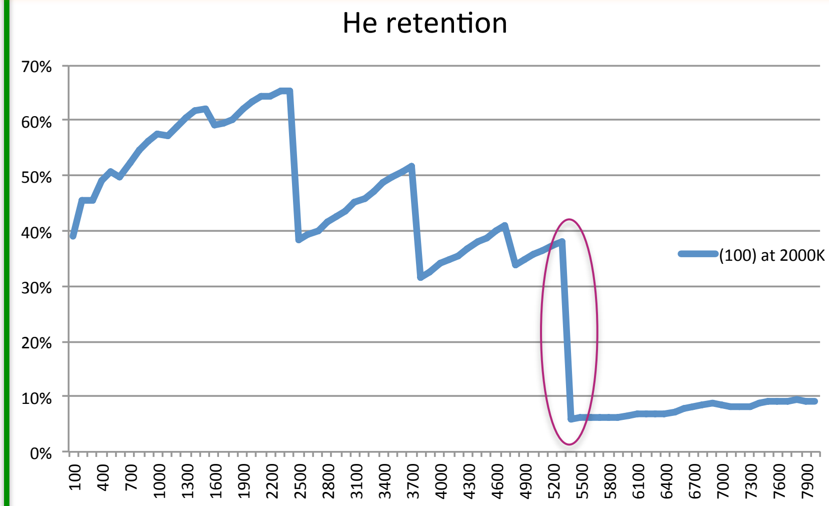


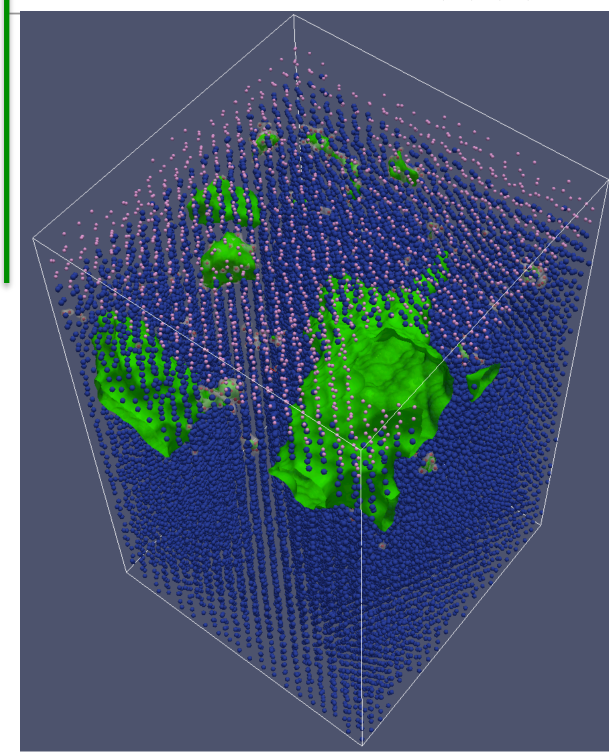
*Bubble growth & bursting: (100) Surface at 2000 K**

Before bubble burst (after 5300 He insertions)
→ 38% He retained

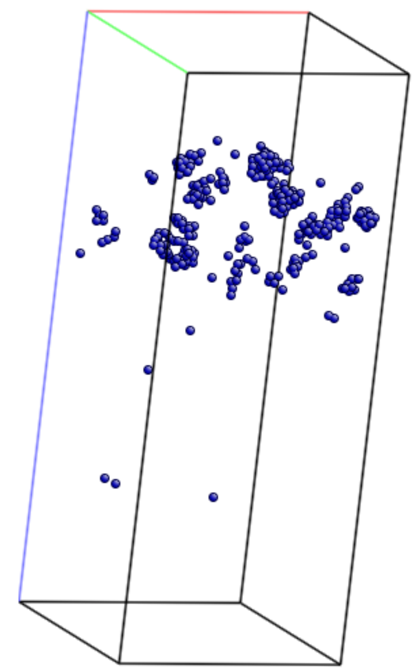


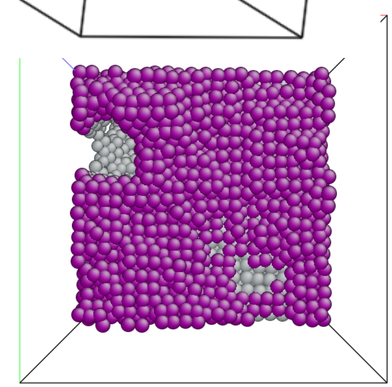






After bubble burst (after 5400 He insertions)
→ 6% He retained

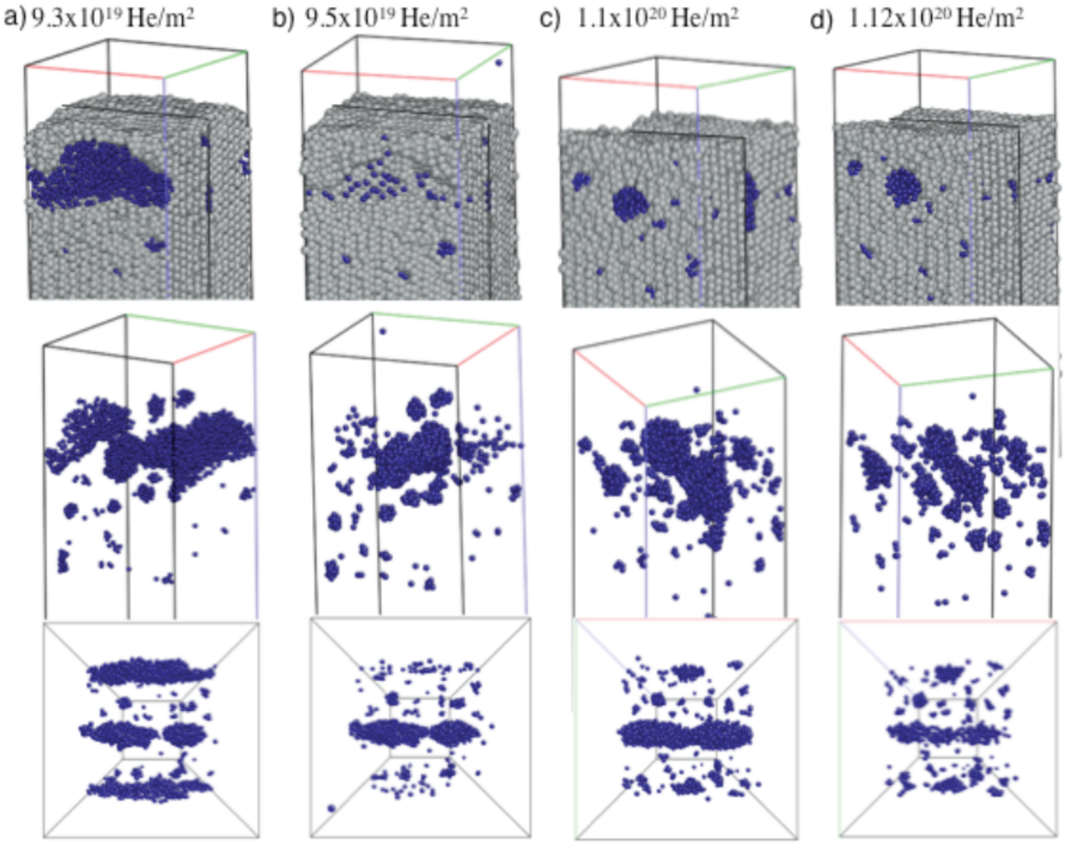


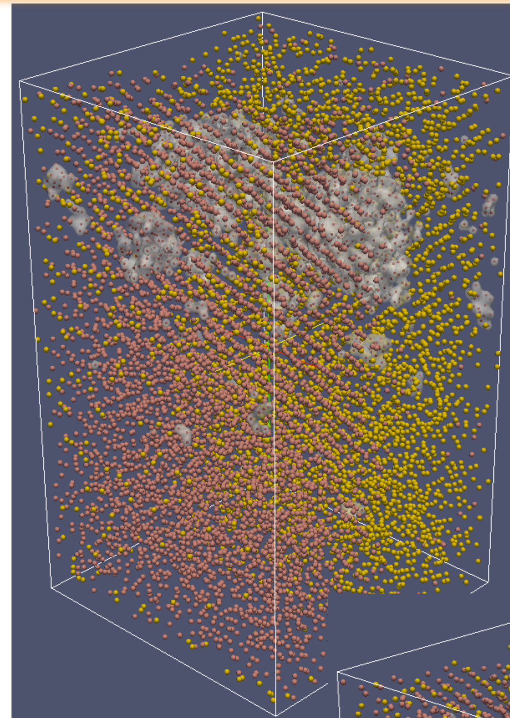


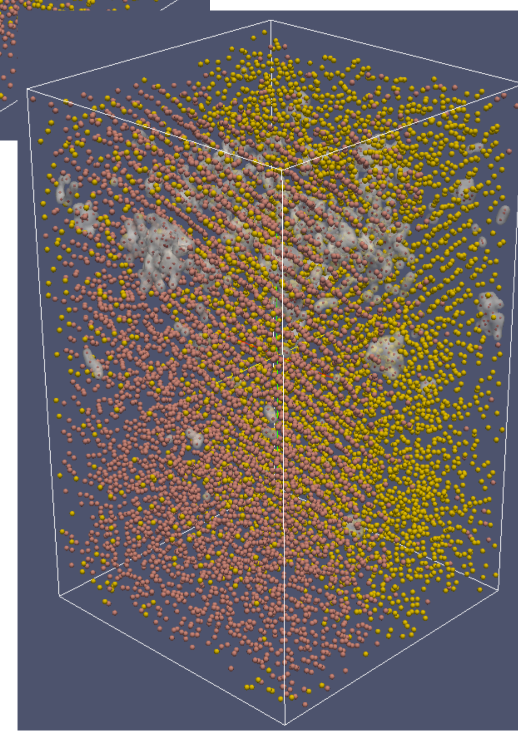
Additional visualization approaches being explored by Ollie Lo (SDAV), which will assist development of alternate model treatments of bubbles (R_o, P, etc)

* Sefta, Hammond, Juslin and Wirth, *Nuclear Fusion* 53 (2013) 073105

Bubble growth & bursting: (100) Surface w Σ5 boundary at 2000 K

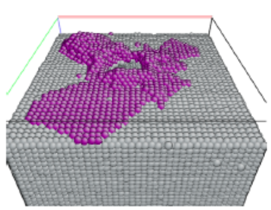




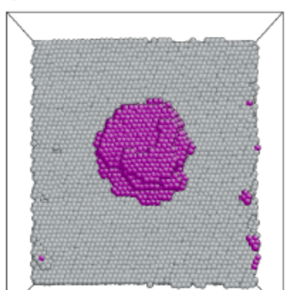


Additional visualization approaches being explored by Ollie Lo (SDAV)

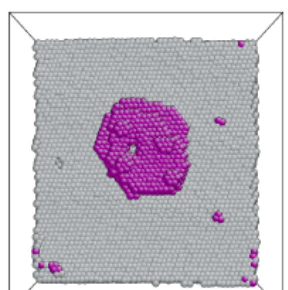
Bubble bursting phenomena is complex* – can crater or self-heal:



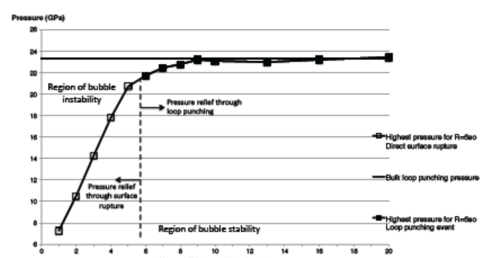
d. Effect of bursting on tungsten surface with previously formed adatom island (d=6 a_o)



c. Closed up surface after first bursting event



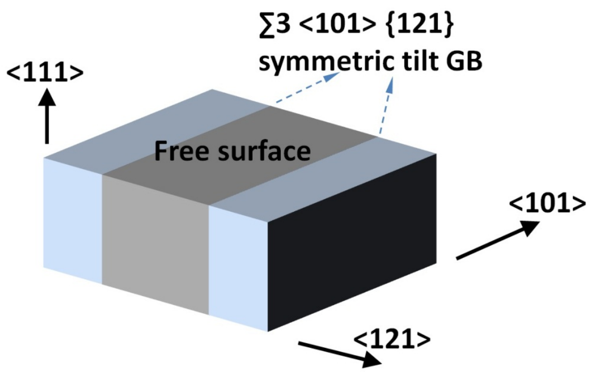
d. Hole after second bursting event



* Sefta, Juslin and Wirth, *JPCM* (2013) submitted.

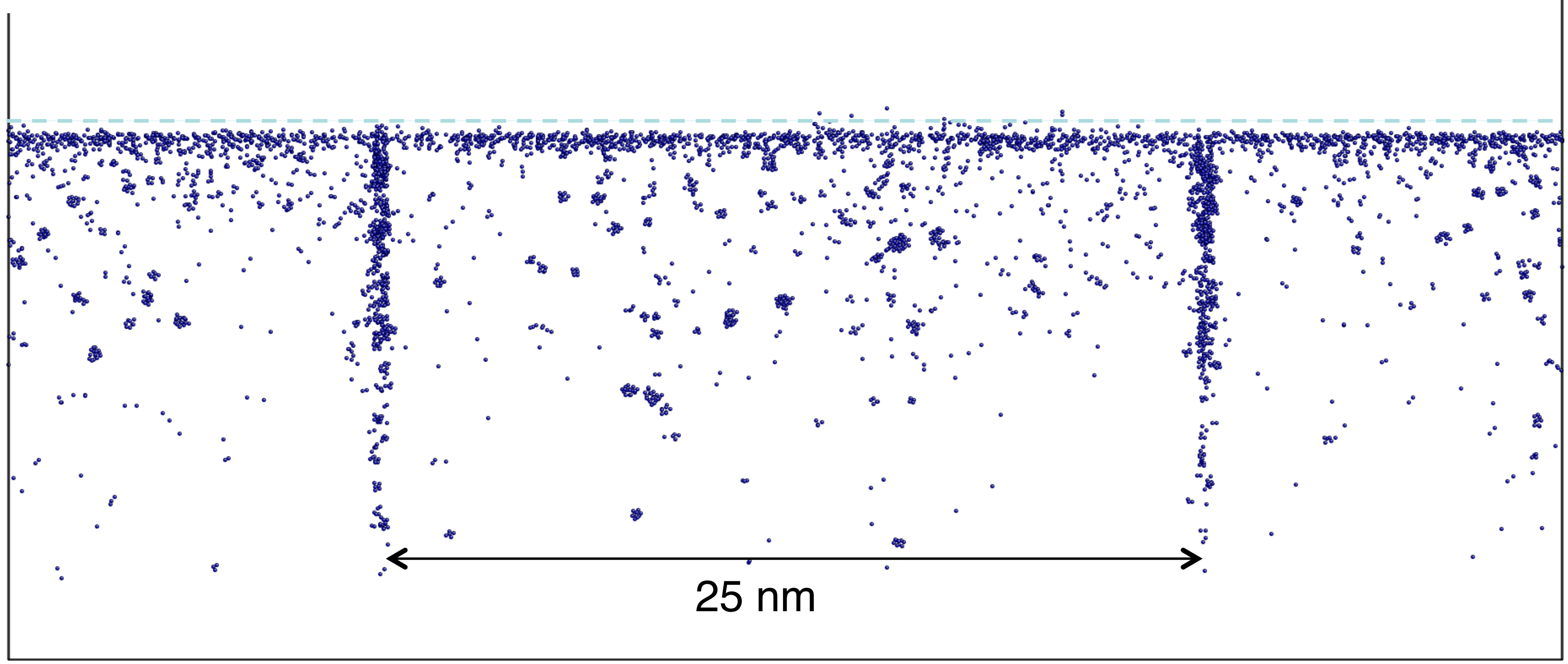
Impact of He implantation flux & temperature

- **Bubble formation, growth by 'trap mutation'/loop punching & bubble bursting identified as key phenomena in smaller scale MD studies, effect of He implantation rate**



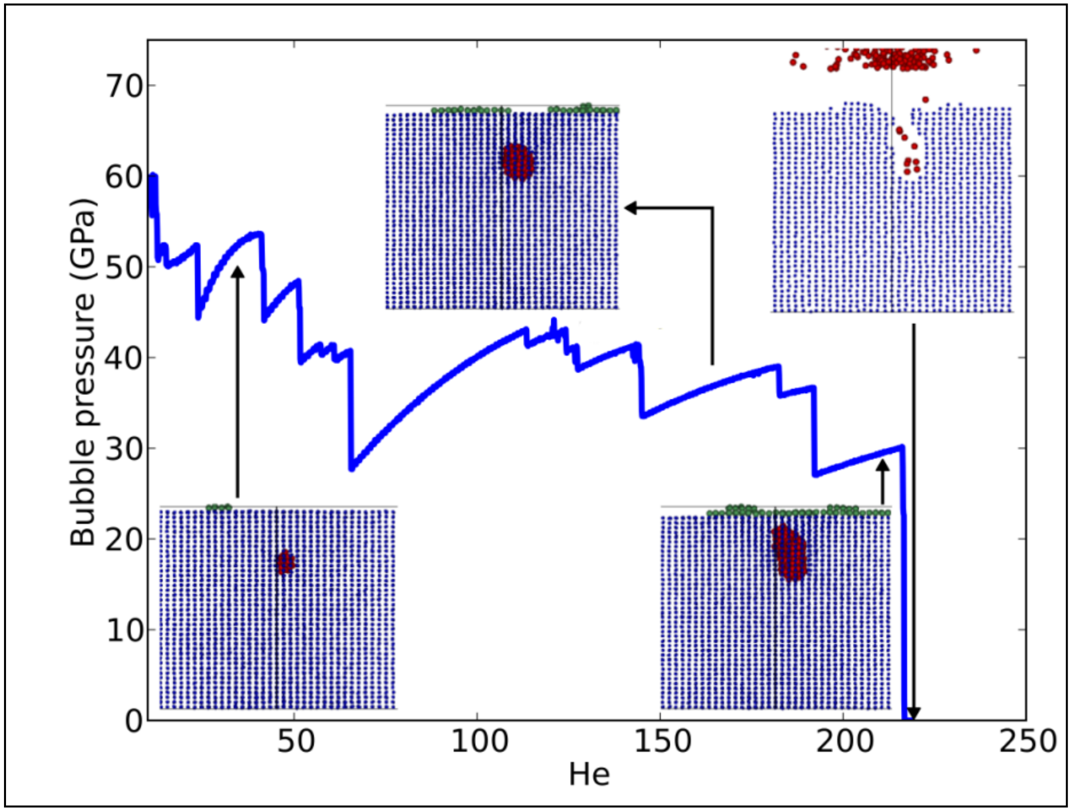
100 eV He implanted at rate of 4×10^{25} He/(m^2-s) at 930 K below (111) surface containing Σ3 grain boundaries

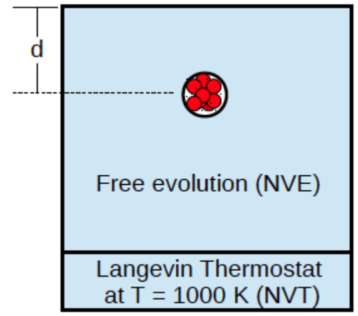
- substantial trapping interaction of grain boundary
- He 'saturation' layer below (111) surface, as well as larger clusters/bubbles forming deeper

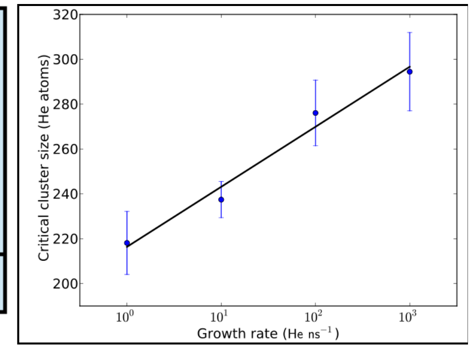


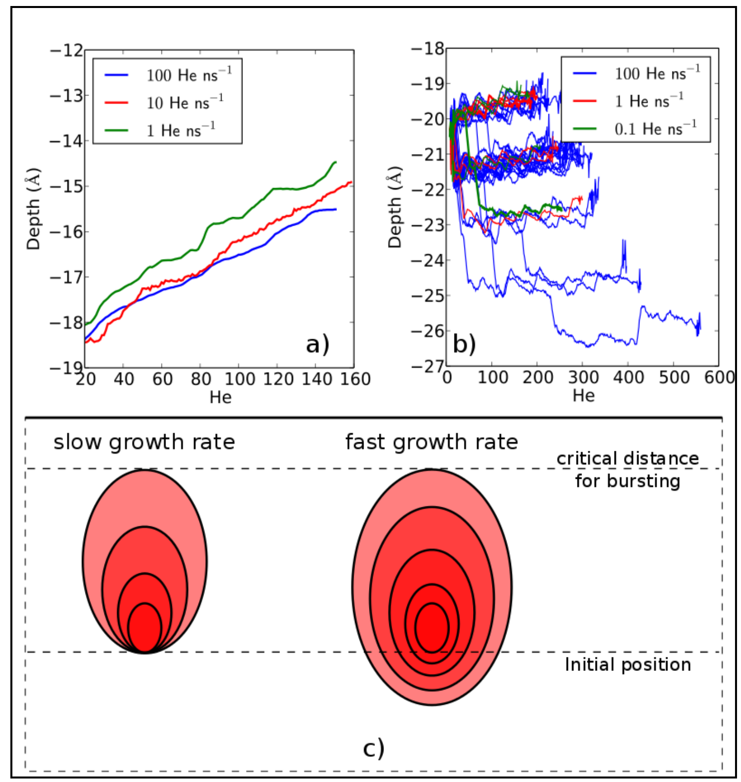
*Impact of He bubble growth rate on rupture**

- **Parallel replica dynamics used to evaluate impact of He bubble growth rate on bubble rupture conditions: Initial 8 He cluster (1.8 nm below surface) simulated with varying rates of He addition to cluster/bubble at 1000 K**









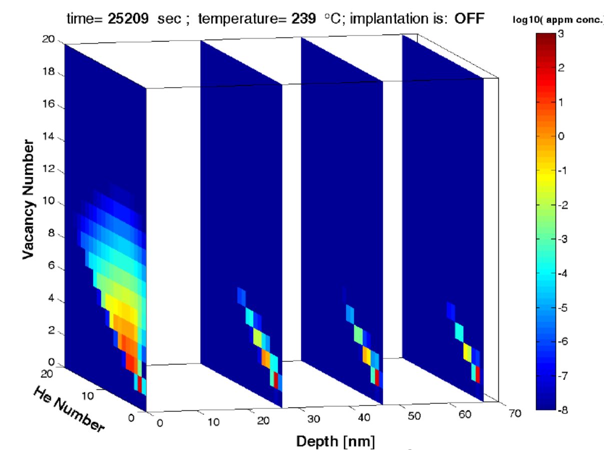
Key phenomena:

- 'trap mutation', loop punching
- surface modification from adatoms/islands
- bubble bursting

* Sefta, Hammond, Juslin and Wirth, *Nuclear Fusion* 53 (2013) 073105; Sefta, Juslin and Wirth, *JPCM* (2013) submitted; Sandoval et al., in preparation

PARASPACE and Xolotl:
Spatially-dependent reaction-diffusion models

Large set of coupled, PDE's that are spatially discretized (Paraspace) and solved using sparse-matrix, implicit time Integration: Future will utilize finite element solutions with

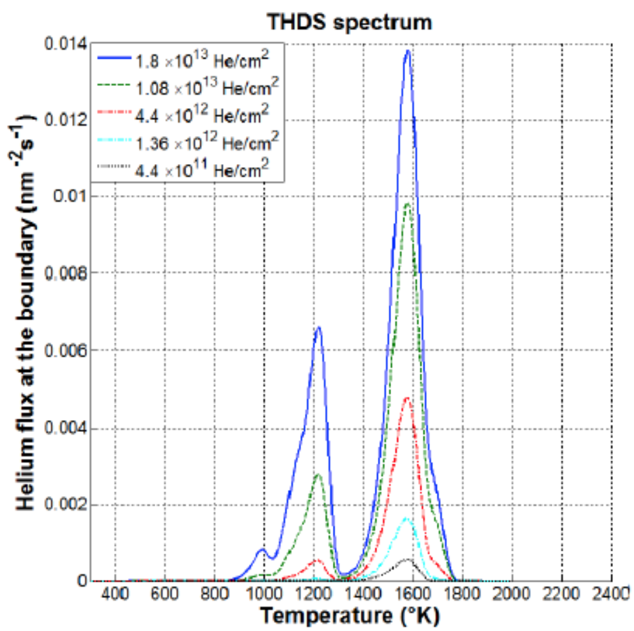


$$\frac{\partial C_i}{\partial t} = P_i(\vec{x}) - \vec{\nabla}\cdot\vec{J}_i + GR_i(\vec{x}) - AR_i(\vec{x}) = P_i(\vec{x}) + \vec{\nabla}\cdot\left(-\frac{D_i\vec{F}}{kT}C_i + D_i\vec{\nabla}C_i\right) + GR_i(\vec{x}) - AR_i(\vec{x})$$

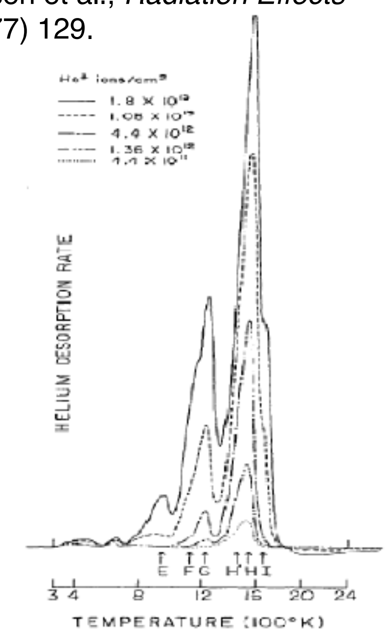
* Reaction events are non-linear (quadratic) but 'local', reaction rate densities described by classical, dilute limit reaction-diffusion theory

* Current approach utilizes finite-difference to obtain large, sparse-matrix which is solved using a linear solver using open-MP & backward difference time integration
* Future: finite element formalism, implicit-explicit (IMEX) ODE solvers and/or differential variational inequality (DVI) solvers in (PETSc)

Simulation & experimental thermal desorption of W irradiated with 5 keV Kr, followed by 250 eV He



Kornelsen et al., *Radiation Effects* **31** (1977) 129.



*Theoretical analysis of He clustering/bubble formation**

• He cluster dynamics described by reaction – diffusion equation in a half-space

$$\frac{\partial C_k}{\partial t} = D_k \frac{\partial^2 C_k}{\partial x^2} + \sum_k KCC + S(x)\delta_{1,k}$$

• Making use of He cluster dynamics
(e.g., fast diffusion of small clusters, trap mutation at k=7)

• Using normalizations:

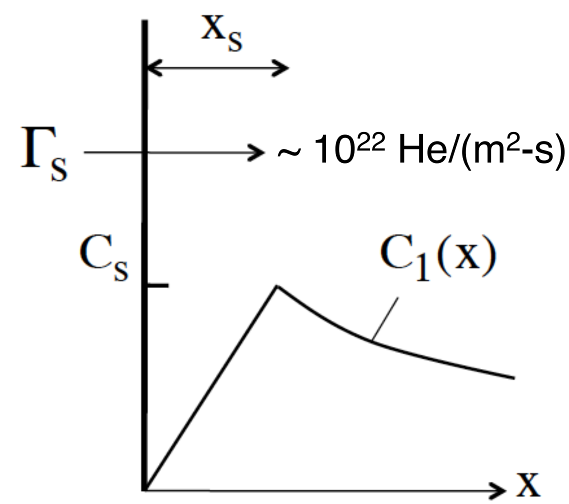
$$\hat{t} = tK_1C_s \qquad \hat{D}_k = D_k/D_1 \qquad \hat{K} = K/K_1$$

$$\hat{x} = x/\ell_{1,1} \qquad \hat{C}_k = C_k/C_s$$

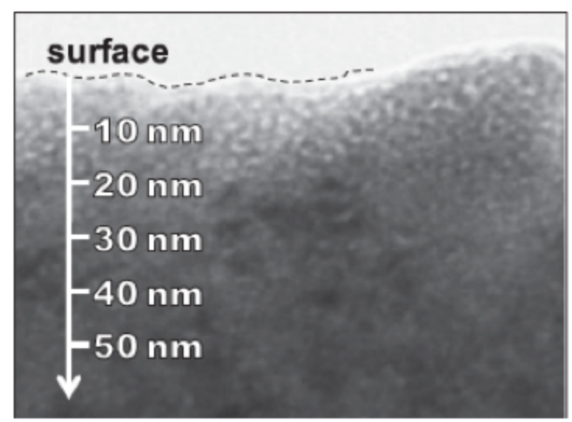
• To obtain reduced set of governing equations:

$$\frac{\partial \hat{C}_k}{\partial \hat{t}} = \hat{D}_k \frac{\partial^2 \hat{C}_k}{\partial \hat{x}^2} + \sum_k \hat{K}\hat{C}\hat{C}, \qquad \hat{C}_k(\hat{x}=0) = \delta_{1,k}$$

which can be assessed theoretically, as well as compared to more detailed numerical simulations



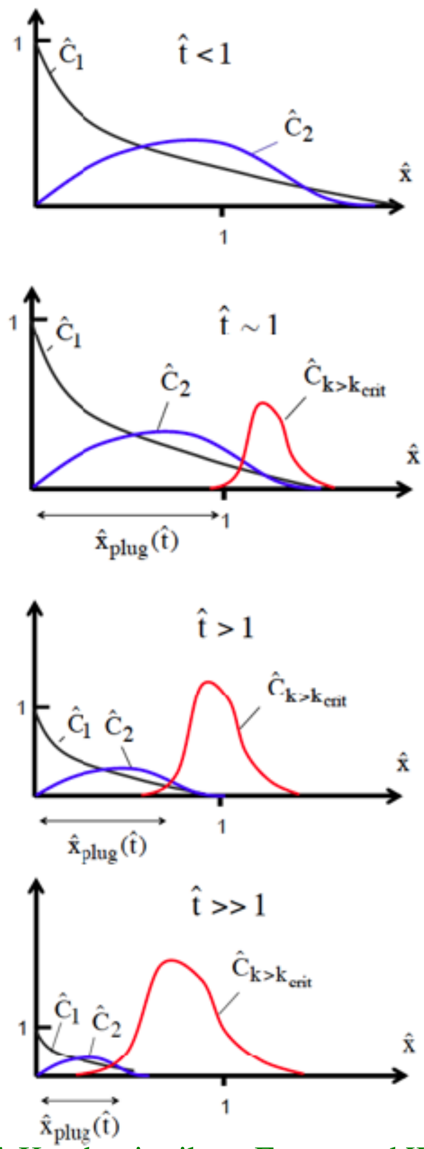
(Miyamoto, 2011)

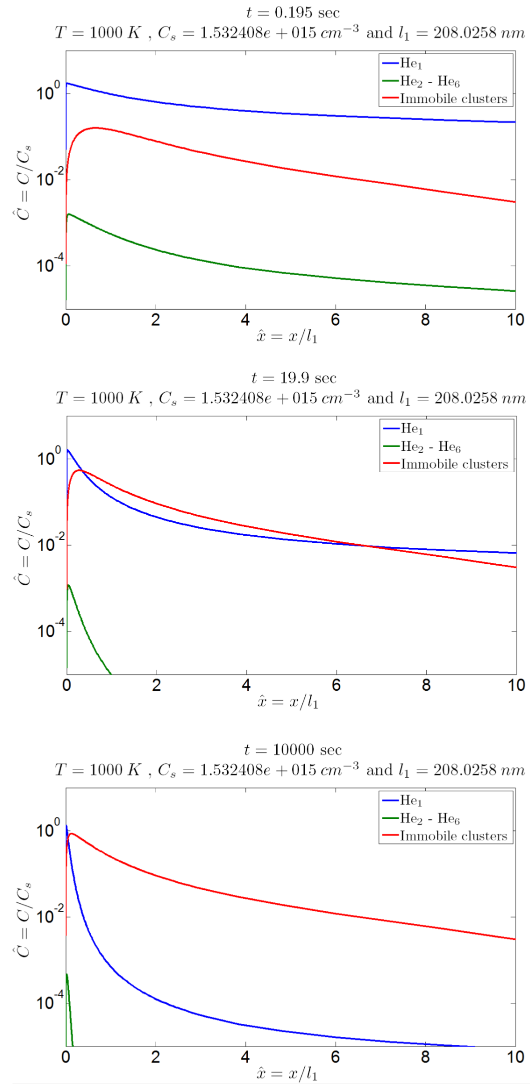


* Krasheninnikov, Faney and Wirth, *Nuclear Fusion* (2013) submitted

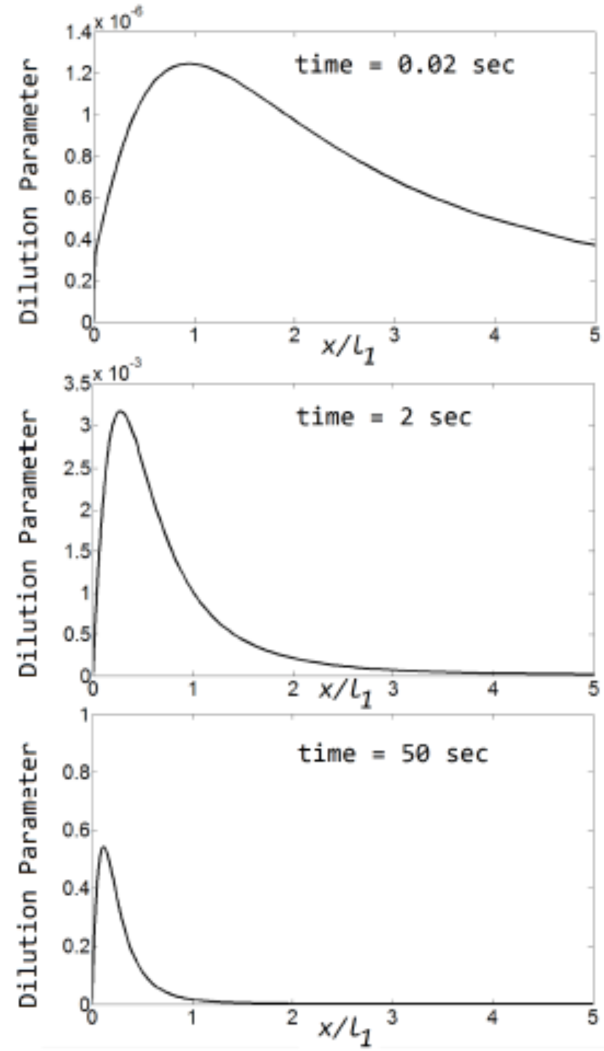
*Theoretical analysis of He clustering/bubble formation**

• Qualitatively, this initiates a 'plug' of helium bubbles that grows towards the surface and blocks deeper diffusion of He – idea supported by detailed numerical simulations





Dilution Parameter = (total He density/W atom density)



However, dilute limit approximation clearly breaks down

* Krasheninnikov, Faney and Wirth, *Nuclear Fusion* (2013) submitted

*Xolotl code**

• Xolotl (SHO-lottle) is the Aztec god of lightning and death
• Developed from 'scratch' for this project, designed for HPC current & emerging architectures (multicore, multicore + accelerator(s))
• Strong engagement with SDAV, SUPER, FastMATH, QUEST during code design and development, thus integrated performance measurement, in-situ analysis & visualization; providing a design with resilience features, checkpoint/research and more

• Leveraging PETSc, MOAB, VisIT and other Institute software

• Developed in C++ with MPI for initial 1D finite difference. 1D and 2D R-z FEM to follow, along with OpenMP, CUDA, OpenCL and OpenACC

• Challenge: Large number of clusters/species (1000's versus 4-5) at each grid point

$$\frac{\partial C_i}{\partial t} = P_i(\vec{x}) - \vec{\nabla}\cdot\vec{J}_i + GR_i(\vec{x}) - AR_i(\vec{x}) = P_i(\vec{x}) + \vec{\nabla}\cdot\left(-\frac{D_i\vec{F}}{kT}C_i + D_i\vec{\nabla}C_i\right) + GR_i(\vec{x}) - AR_i(\vec{x})$$

$$GR_i(\vec{x}) = \sum_{\substack{jk \\ j+k=i}} k^+_{jk}C_jC_k + \sum_j k^- C_j \qquad AR_i(\vec{x}) = C_i\sum_j k^+_{ij}C_j + k^- C_i$$

- Most species only involved in reactions (off diagonal blocks) but local
- Requires highly accurate Advection-Diffusion-Reaction (ADR)
- Large-scale nature of 3D, ITER divertor PSI problem, $O(10^3 x 10^3 x 10^3 x 10^4)$ requires HPC to Exascale computing

* Xolotl Web Site: https://sourceforge.net/projects/xolotl-psi/

Xolotl – FASTMath interaction developing solution methods

Solution strategy: Solved with implicit or semi-implicit ODE integrator, Newton based non-linear solver and multi-grid based linear solver
- Leverages ODE IMEX infrastructure in PETSc
- Links to hypre multigrid solvers

Outstanding questions:
- Large, but sparse matrix of reaction terms may be leveraged (GPUs?) – optimal parallelization strategy remains to be determined
- Unclear whether standard multigrid will be sufficient for highly accurate solutions

• Strong interaction developed in Dec 2012, after Xolotl math document* was finalized, and PETSc team developed ADR solver protoype (our Christmas miracle) --- very strong interactions continue on solver issues and code design

• MOAB – PETSc integration within FASTMath will be heavily leveraged and engaged in transitioning Xolotl 1D finite difference to 1D & 2D (R-z) FEM

* https://docs.google.com/document/d/1Ssm3gja35IeGsCxcZoKcAHOOGUf7S_4sV3DbKooSEt8/edit?usp=sharing

Xolotl – QUEST interactions

Following participation in QUEST annual meeting (April 2013), Xolotl team began close engagement with QUEST to further develop appropriate UQ strategy

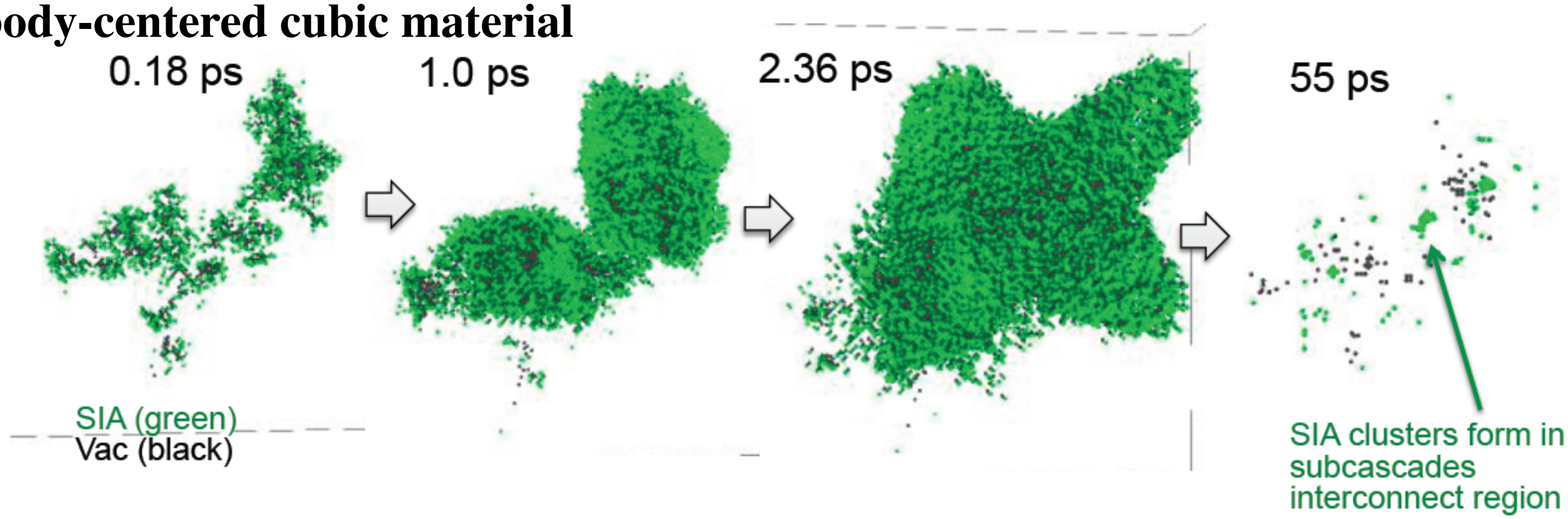
Initial ideas involved intrusive UQ using adjoint analysis – However significant implementation challenges because of canards within our ADR system (e.g., strongly exponential diffusivities)

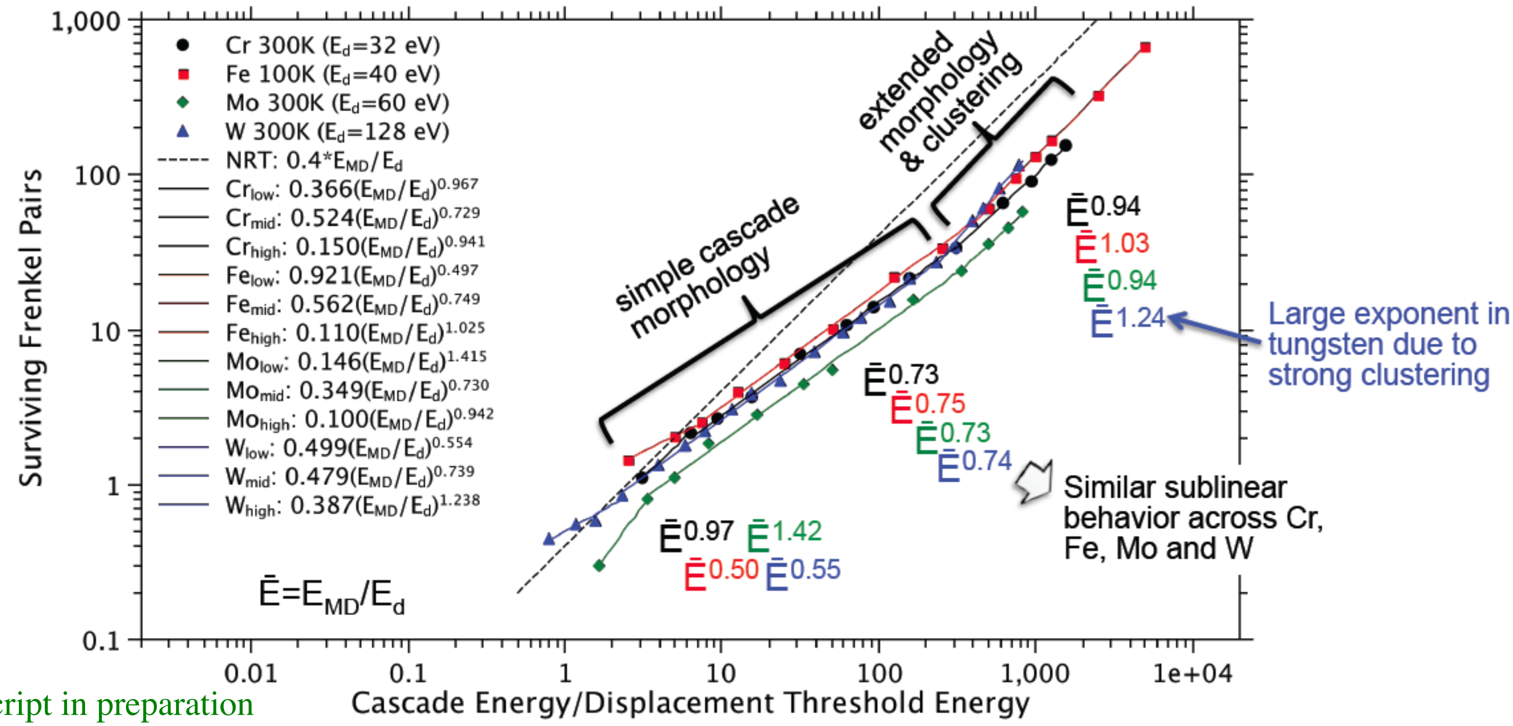
QUEST review of Xolotl math document* resulted in a comprehensive strategy we are pursuing jointly with QUEST to perform non-intrusive UQ using DAKOTA and QUESO

* https://docs.google.com/document/d/1Ssm3gja35IeGsCxcZoKcAHOOGUf7S_4sV3DbKooSEt8/edit?usp=sharing

*14 MeV neutron damage in bulk tungsten**

- **Large database of defect production in energetic displacement cascades developed in tungsten and body-centered cubic material**



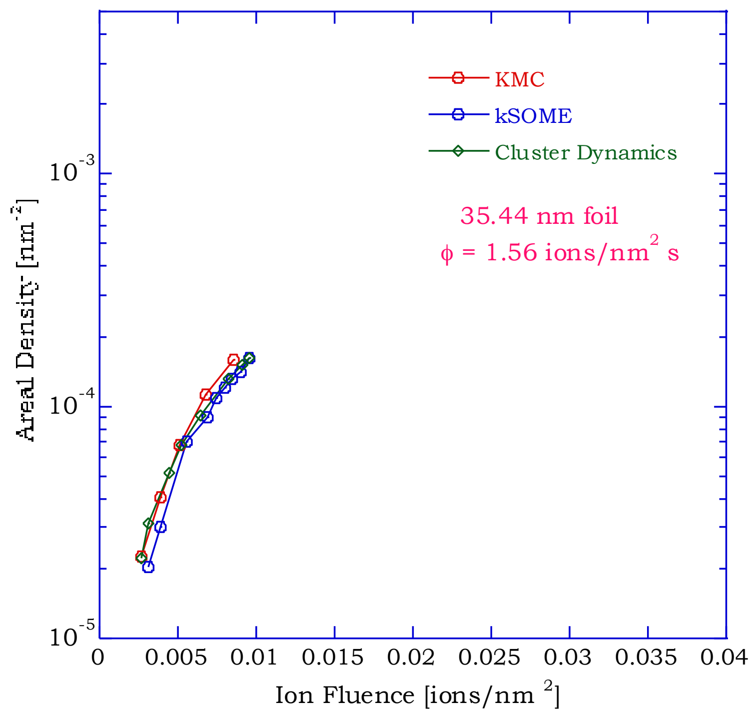


* Setyawan et al., manuscript in preparation

Kinetic Monte Carlo simulations: kSOME

- **kSOME code under-development at PNNL (Nandipanti, Roche and Kurtz) 'Object' Monte Carlo codes in materials science are traditionally sequential/single processor. Ken Roche working on optimizing algorithm and parallelization:**

- Identified unstructured I/O and related data tracking to improve performance
- Initial parallelization focused on threaded approach to update reaction tables simultaneously (rather than sequentially): Strong scaling realized
- Optimization demonstrated that 320 nm x 320 nm x 35 nm simulation cell simulated to 4 seconds during 1 MeV Kr ion irradiation of thin foils which requires 160 Million MC steps went from 52.5 hours CPU time (original) to 32.5 hours (CPU + box method data tracking + pthreads) & verified against other methods*
- Implemented prototype kSOME with mutually inclusive parallel execution modes:
    - Distributed memory over distinct configurations;
    - Distributed memory within particular configurations
    - Shared or distributed memory update evolving defects
- Experimenting with improved table queries and defect evolution for GPU



* Xu, Hu and Wirth, *Applied Physics Letters* **101** (2012) 101905; Xu, Wirth, et al., *Acta Mater* **60** (2012) 4286

Summary & Future Challenges

• Strong interactions within team & with SciDAC Institutes

• Initial discovery science to provide mechanistic understanding of W surface dynamics under low-energy He plasma exposure & initial integration with experimental efforts

- Characterized thermodynamics/kinetics of small He clusters
- Discovery of surface topological changes (ad-atom, loop punching, bursting) & He bubble evolution using MD
- Initial MD/AMD studies to evaluate rate effects on He agglomeration kinetics (10^{27} to $4x10^{25}$ He/(m^2-s)) and bubble growth/burst mechanisms (10-10^3 He/ns)
- Theoretical analysis indicates need to go 'beyond the dilute limit'
- Development of new KMC code (kSOME) & continuum PSI simulator (Xolotl); strong engagement with Performance/Optimization, (SUPER), ADR solvers in PETSc (FASTMath), SDAV & QUEST
- Next steps for Xolotl move to FEM & engage MOAB (FASTMath)

• Successful completion of the project (2017) will provide simulation tools to evaluate tungsten-based plasma facing component and divertor components in a burning plasma environment.