SciDAC – PSI (Plasma Surface Interactions): Present and Future Computing Requirements

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SciDAC-PSI project description

• Focus on plasma materials interaction (PMI) encompassing 3 coupled spatial regions:
- Edge/scrape-off-layer region of the plasma (X. Tang, J. Canik);
- Near surface material response to extreme thermal & particle fluxes under the influence of, and feedback to, the plasma sheath (B.Wirth, B. Uberuaga and D. Maroudas); and
- Structural materials response to intense, 14 MeV-peaked neutron spectrum (R. Kurtz)

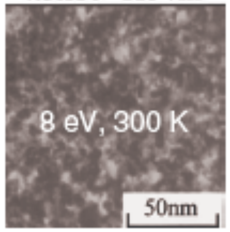
• Utilize both particle-based and continuum approaches to develop & deploy validated, high performance simulation tools for these distinct spatial domains, and develop techniques for multiscale integration and interfacing across these domains

• 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. More specifically:
- What physical parameters control the time dependent evolution of the near-surface morphology and composition of the re-deposition layer – key phenomena to model include recycling, surface morphology, gas bubble, precipitate and second phase domains (including porosity), and gas fueling/recycling
- What are the effects of high-energy neutron damage on mediating, or exacerbating, near-surface defect evolution and tritium species permeation and retention?
- What is the impact of dilute impurities (O, Be, …) on surface morphology evolution and plasma contamination and how does mixed material transport in tokamaks impact erosion and impurity generation?
- How does the evolving bulk microstructure impact the thermal properties, and thereby feedback into PFC evolution by modifying the resulting temperature profiles?

W Surface dynamics under combined thermal/particle fluxes

T < 700 K

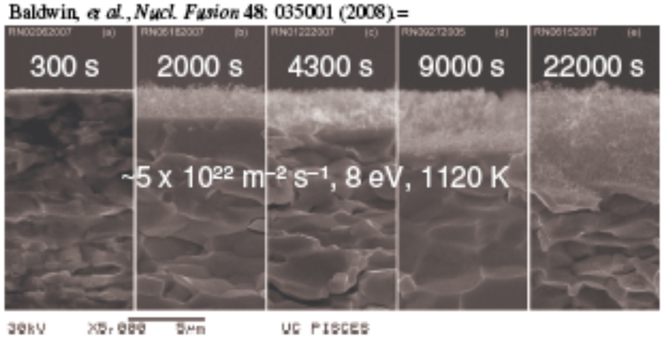
$4.3x10^{19}He^+/m^2$



H. Iwakiri, *et al., J. Nucl. Mater.* 283–287: 1134–1138 (2000).

non-specific damage

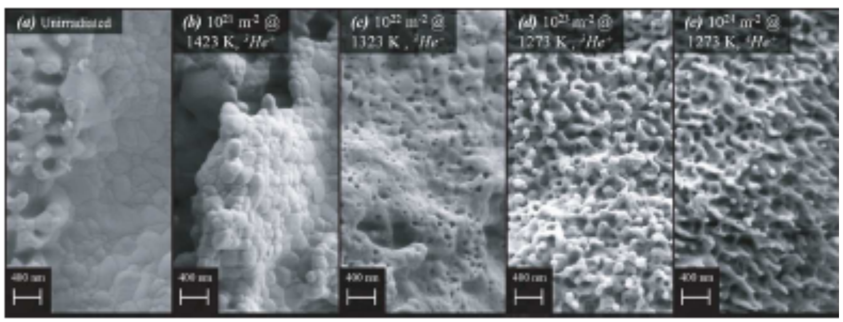
Baldwin, *et al., Nucl. Fusion* 48: 035001 (2008).



900 K < T < 1900 K

fuzz / coral

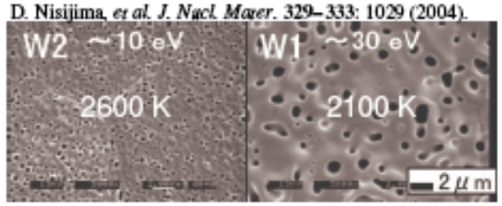
S. J. Zenobia and G. L. Kulcinski. *Phys. Scr.* T138: 014049 (2009).

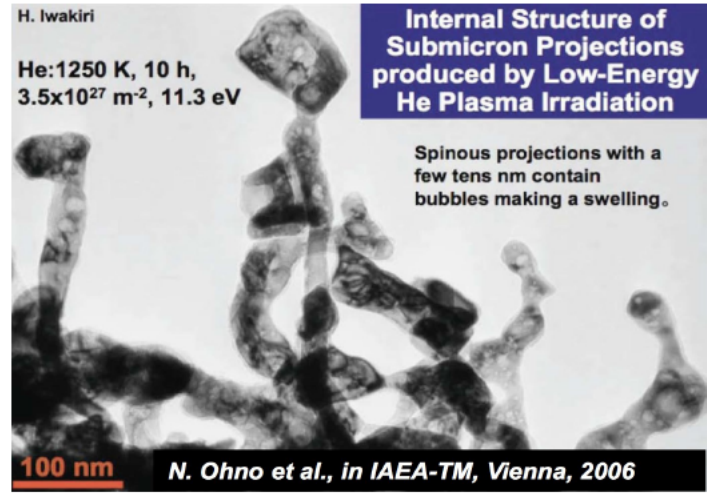


T > 2000 K

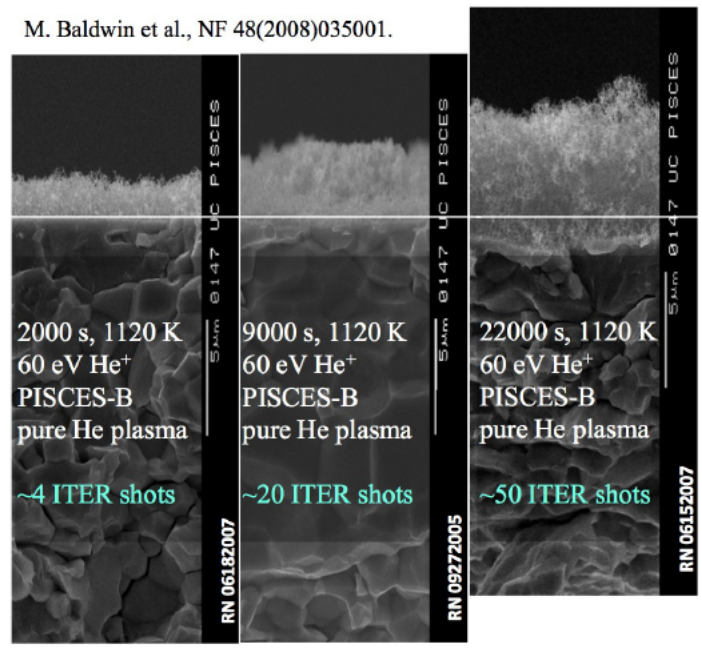
holes

D. Nisijima, *et al. J. Nucl. Mater.* 329–333: 1029 (2004).





M. Baldwin et al., NF 48(2008)035001.



*Complex, interlinked PSI phenomena**

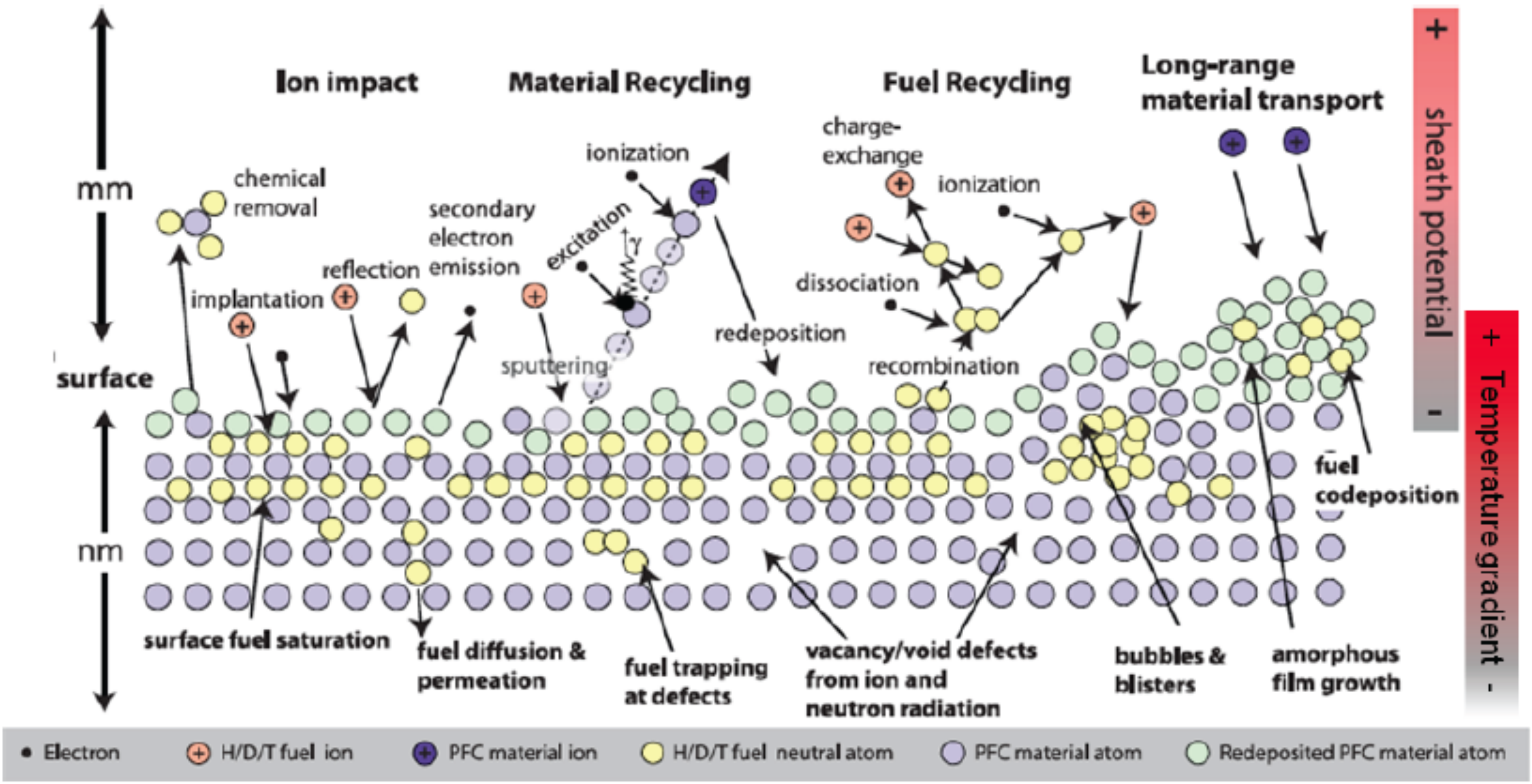


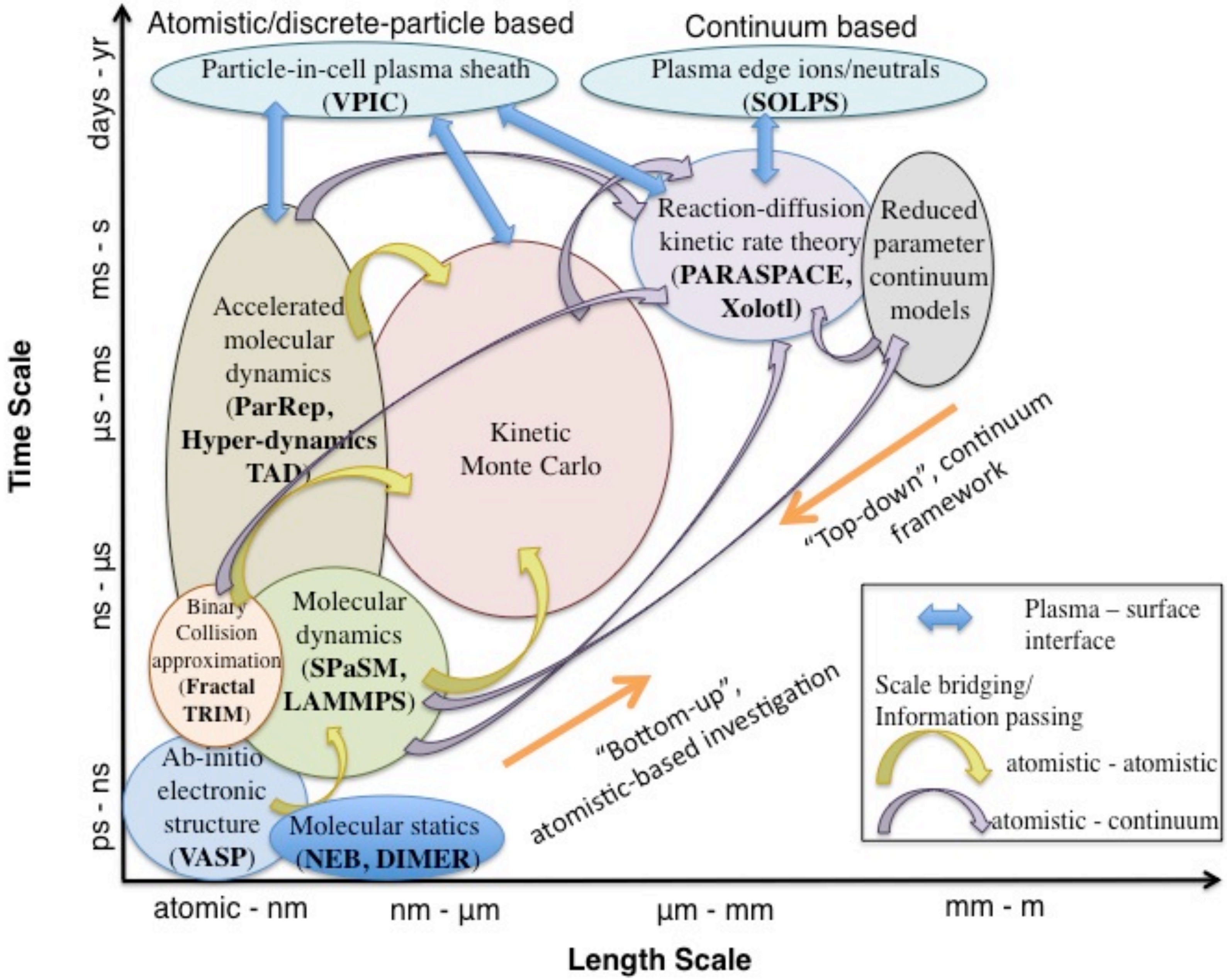
Figure of merit:

Incident plasma ion flux near divertor strikepoint: 10^{24} $m^{-2}s^{-1}$

Steady-state sputtering yield O (10^{-4}) on surface monolayer (10^{19} atoms/m^2) results in sputtering of every atom every 0.1 sec -> every atom sputter >10^8 times/year

* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

SciDAC-PSI computational strategies



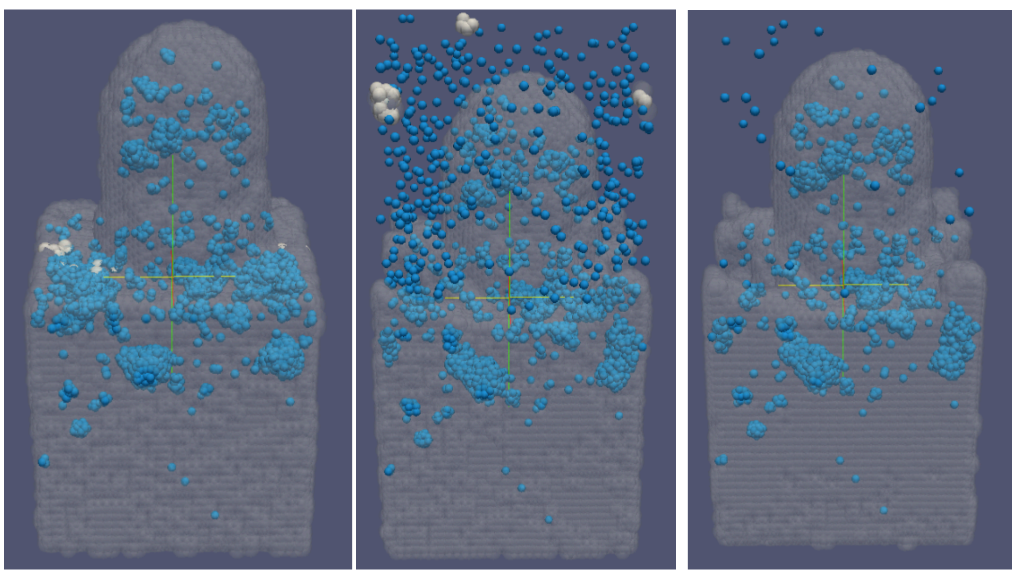
Molecular Dynamics calculations

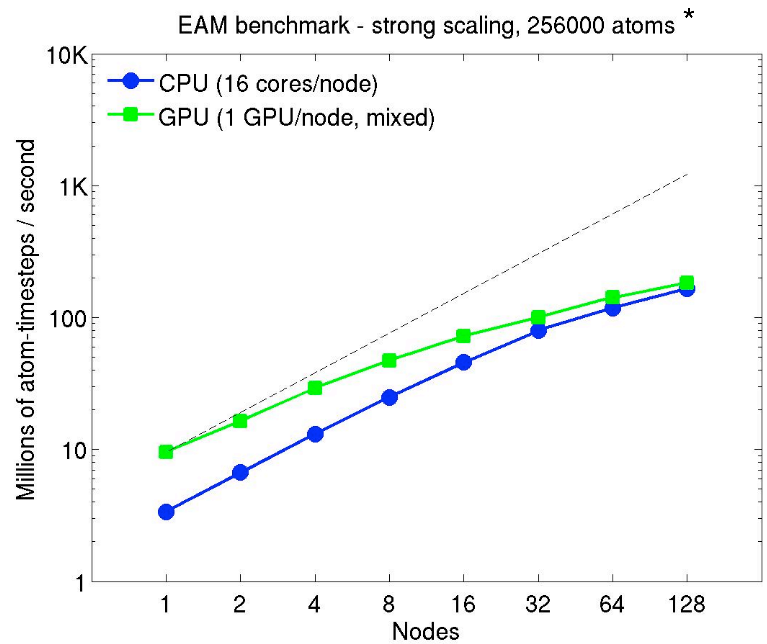
- **'Common' MD codes: LAMMPS, SPASM**

- typically run on small clusters/small atomistic domains (usually because of throughput), especially for 'discovery' science
- LANL has demonstrated SPASM for 1 billion atoms for 1 nanosecond
- LAMMPS has been demonstrated on GPUs/TITAN

- **Accelerated MD codes – PRD has been run on roadrunner over 12,000 replicas**

Road Runner experience (PRD):
Flop count: petaflop
number of cores: 120,000
wall clock time: 24 hours
total memory: 12000 GB
minimum memory per core: 0.1 GB
total data read & written per run: 100 GB
size of checkpoint file: 0.1 GB





* http://lammps.sandia.gov/bench.html#titan

Kinetic Monte Carlo simulations

- **kSOME code under-development at PNNL (Kurtz and Roche)**

'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 effort focused on threaded approach to update reaction tables simultaneously (rather than sequentially): Current strong scaling realized**

- **Planned parallel version of kSOME will allow mutually inclusive models of parallelization:**
  - **Distributed memory over distinct configurations;**
  - **Distributed memory within particular configurations**
  - **Shared or distributed memoy over update of evolving defect configuration**

- **Current performance optimization has 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)**

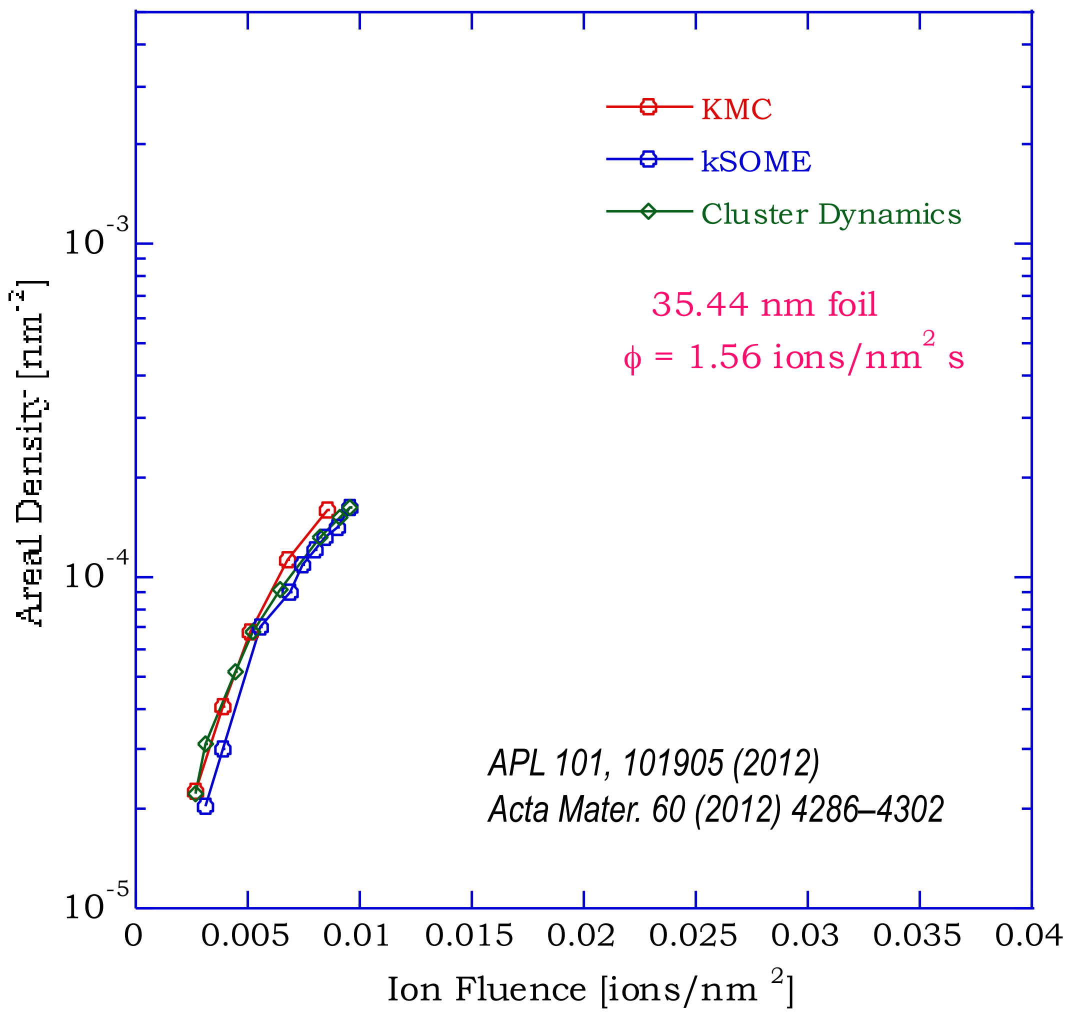
Kinetic Monte Carlo simulations

Irradiation conditions:

- System Size = 315 nm x 315 nm x 35.44 nm
- 1 Mev Kr ion irradiation at 80 ˚C

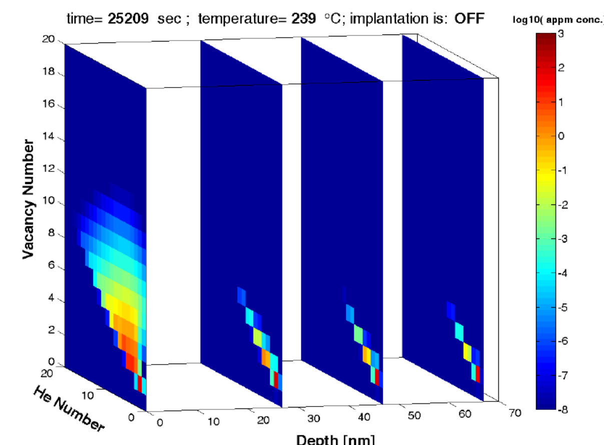
Other code improvements (K. Roche):

- A suite of profile benchmarks on Titan completed
- Experimented with asynchronous communication tests and mixed mode MPI + threads on Titan nodes for several basic operations



PARASPACE/Xolotl-PSI: 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



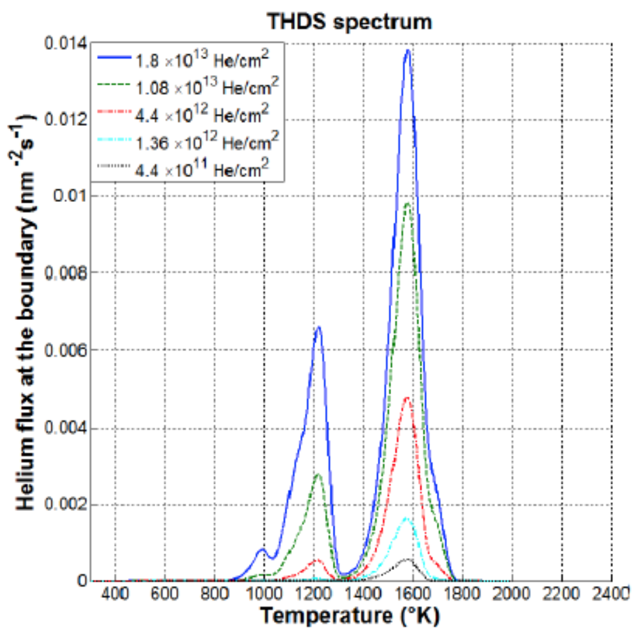
$$\frac{\partial C_i}{\partial t} = P_i(\vec{x}) - \vec{\nabla}\cdot\vec{J}_i + GR_i(\vec{x}) - AR_i(\vec{x}) = P_i(\vec{x}) + \vec{\nabla}\cdot\left(-\frac{D_i\vec{F}}{kT}C_i + D_i\vec{\nabla}C_i\right) + GR_i(\vec{x}) - AR_i(\vec{x})$$

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

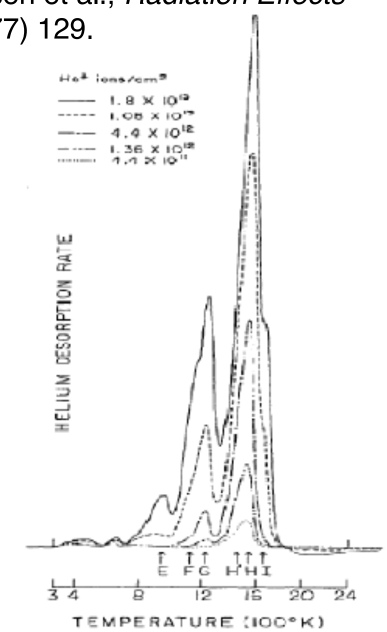
* Current approach utilizes finite-difference to obtain large, sparse-matrix which is solved using a linear solver using open-MP & backward difference time integration

* 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.



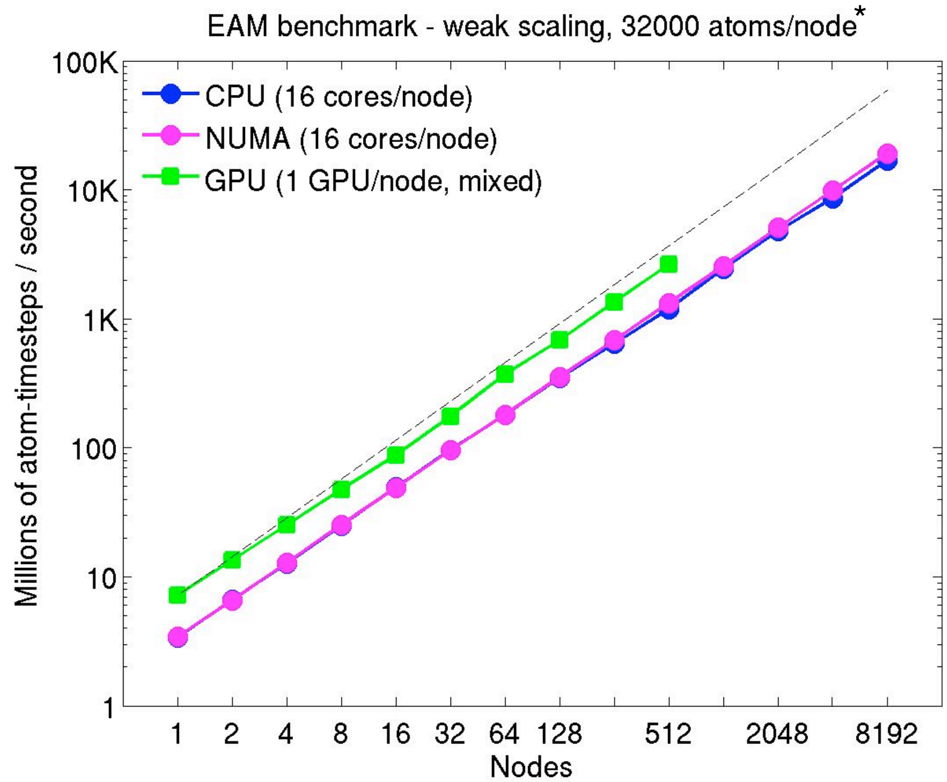
Current HPC Usage

- m1709 (SciDAC-PSI) is new 2013 repository – envision 5M cpu hours in 2013
  - m1200 (atomistics of plasma surface interactions) used ~0.4M cpu hours in 2013

Anticipated 2013 MD/AMD runs:

- ~80 total simulations for 10 million atoms for approximately 10 ns (MD/ LAMMPS) (256 cores) - requires ~10 queue submissions/checkpoints
- ~20 total simulations consisting of 50 million atoms for approximately 10 ns (MD/LAMMPS) (1024 cores)
- ~20 Accelerated MD simulations for 10 million atoms for approximately 1 ms

- kSOME (KMC) optimization and testing



* http://lammps.sandia.gov/bench.html#titan

HPC requirements for 2017 & new architectures

- Xolotl-PSI currently being written/coded, based on a finite element implementation of the reaction-diffusion problem, coupled to PETSc solvers and including intrinsic code performance and uncertainty quantification ‘hooks’, as well as flexibility for HPC computing infrastructure (e.g., GPUs or other large-scale single-instruction, multiple-data oriented processors)
  - Details of code & performance/scaling remain to be determined

- 3 Dimensional modeling of surface response to plasma with cross-sections on the scale of mm^2 to cm^2 and depth of several microns constitutes a problem on the scale of $O(10^{12}\text{-}10^{13})$ unknowns. The need for long time integration (> 2 years of radiation damage) requires the ability to use large time steps and inexpensive time steps – anticipate use of IMEX solvers but still much remains unknown.

- Estimate of specific details of compute hours, memory, concurrency will be provided in case study document

Summary & Future Challenges

• Performance of plasma facing components (PFCs) and materials is an inherently multiscale challenge – significant effort ongoing to utilize multiscale materials modeling and high performance computing – but this is in the very early stages of research and implementation – lots of effort at different scales, few (none) integrated codes using high-performance computing

• Continued 2x/year increases in HPC capability can be expected to drive understanding of the passing of information across particle-based simulation techniques (e.g., multiscale integration) and enable large-scale, continuum level simulations of surface topology, chemistry and gas inventory during steady-state PFC operation in ITER-like conditions