July 12, 2022

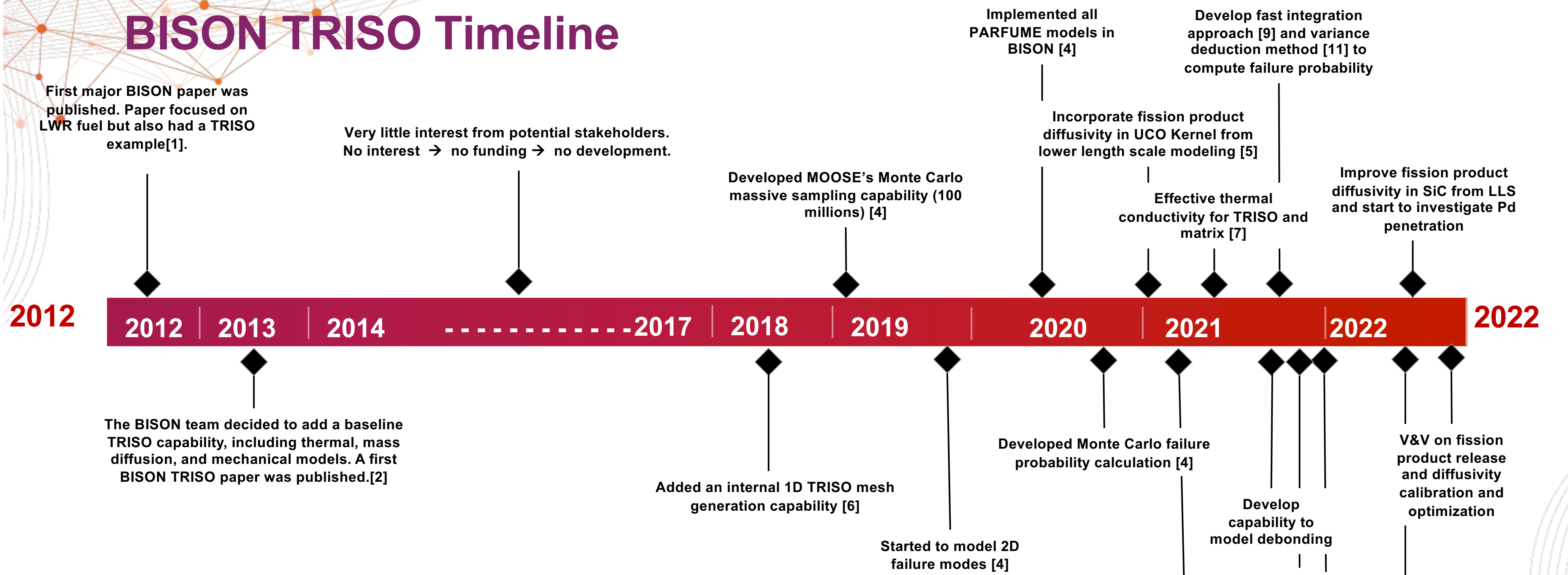
Wen Jiang

TRISO Fuel Performance Modeling with Bison

ART Advanced Reactor Technologies

GAS-COOLED REACTORS

BISON TRISO Timeline



[1] R.L. Williamson et al, Multidimensional multiphysics simulation of nuclear fuel behavior, JNM, 2012

[2] J.D. Hales et al, Multidimensional multiphysics simulation of TRISO particle fuel, JNM, 2013

[3] R.L. Williamson, et al, Bison: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms, NT, 2020

[4] W. Jiang et al, TRISO particle fuel performance and failure analysis with BISON, JNM, 548, 152795, 2021

[5] X.Y. Liu et al, Atomistic and cluster dynamics modeling of fission gas (Xe) diffusivity in TRISO fuel kernels, JNM, 561, 153539, 2022

[6] J.D. Hales et al, Modeling fission product diffusion in TRISO fuel particles with BISON, JNM, 548, 152840, 2021

[7] A. Toptan et al, FEA-aided investigation of the effective thermal conductivity in a medium with embedded spheres, NED, 381, 2021

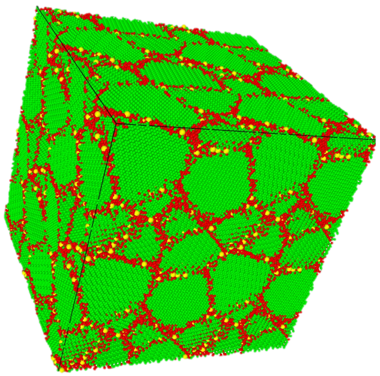
[8] J. D. Hales, et al, Numerical Evaluation of AGR-2 Fission Product Release, JNM, 558, 153325, 2022

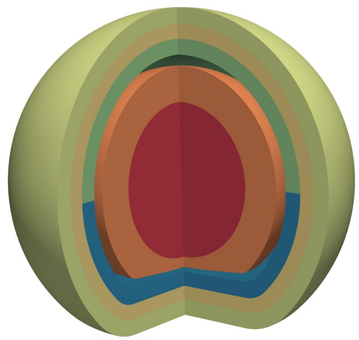
[9] W Jiang, et al, Efficient High-Fidelity TRISO Statistical Failure Analysis using Bison: Applications to AGR-2 Irradiation Testing, JNM, 153585, 2022.

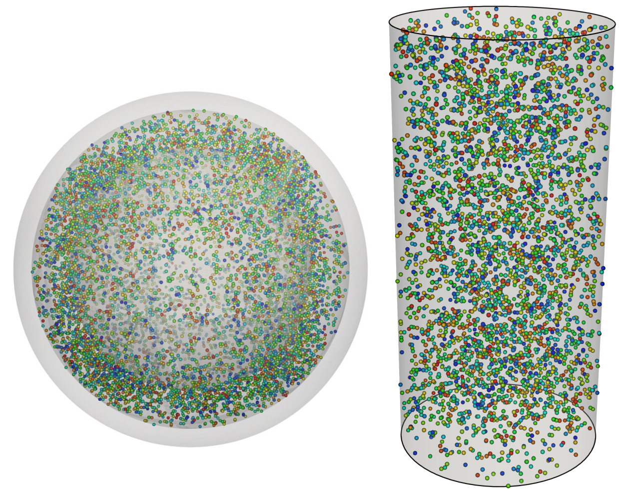
[10] P.-C. A. Simon et al., Mechanistic calculation of the effective silver diffusion coefficient in polycrystalline silicon carbide: application to silver release in AGR-1 TRISO particles, JNM, 153669, 2022

[11] S.L.N. Dhulipala et al, Accelerated Statistical Failure Analysis of Multifidelity TRISO Fuel Models, JNM, 153604, 2022

Multi-scale TRISO Modeling Overview







Lower-length scale modeling

- **Fission gas release model:** Xe, Kr diffusivity in UCO
- **Fission product diffusivity:** Silver diffusion in SiC, Pd Penetration

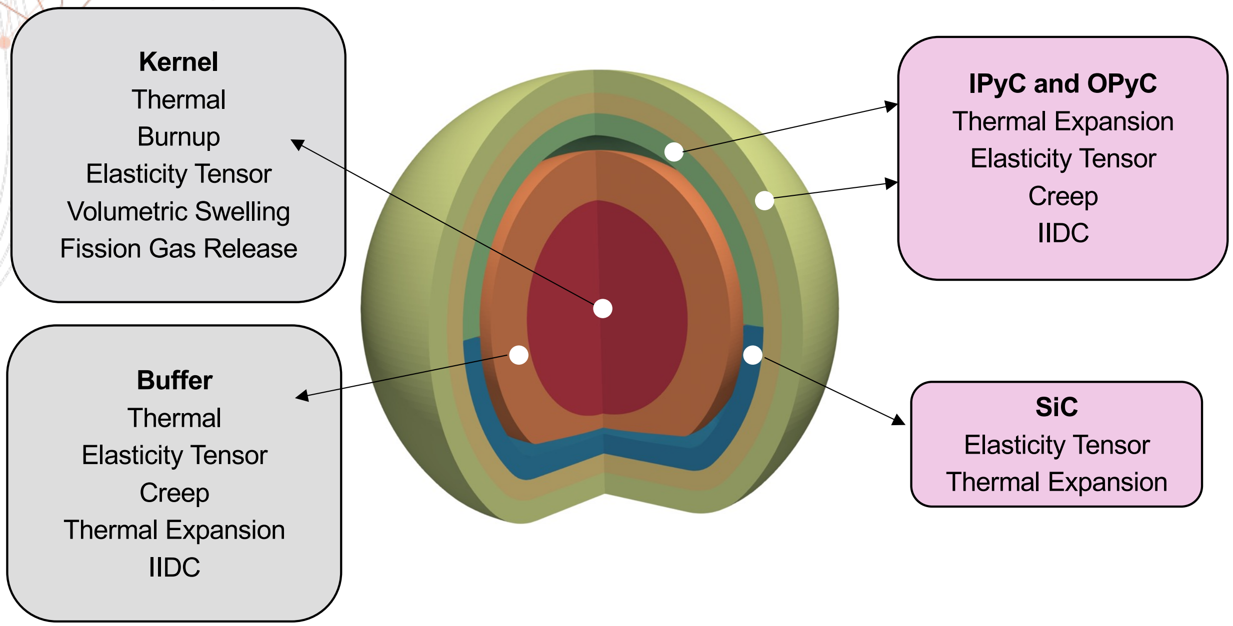
TRISO particle

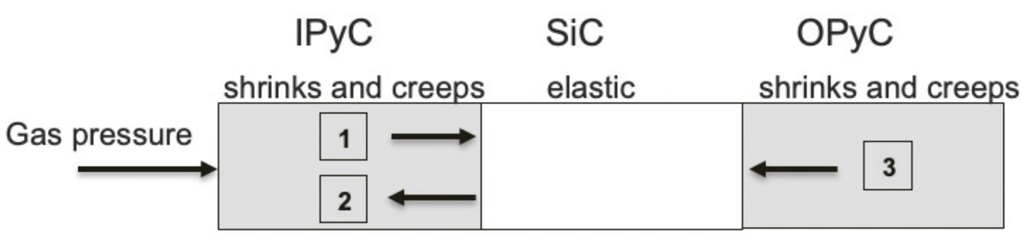
- **Thermal-mechanical modeling**
  - **Failure analysis:** asphericity, IPyC cracking and debonding
- **Fission product diffusion through layers**

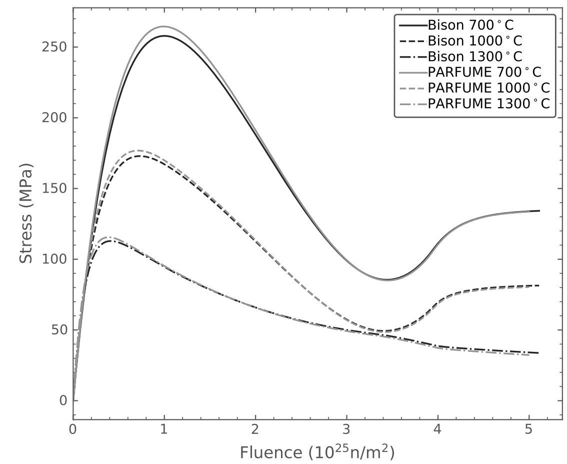
Pebble and Compact modeling

- **Failure probability calculation**: Monte Carlo and Fast Integration Approach
- **Fission product diffusion through matrix**
- **Particle-Matrix interaction**

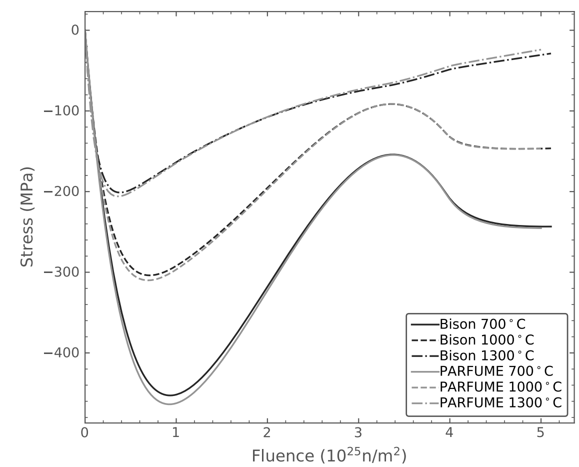
TRISO Fuel Particle Modeling







Tangential stress in IPyC

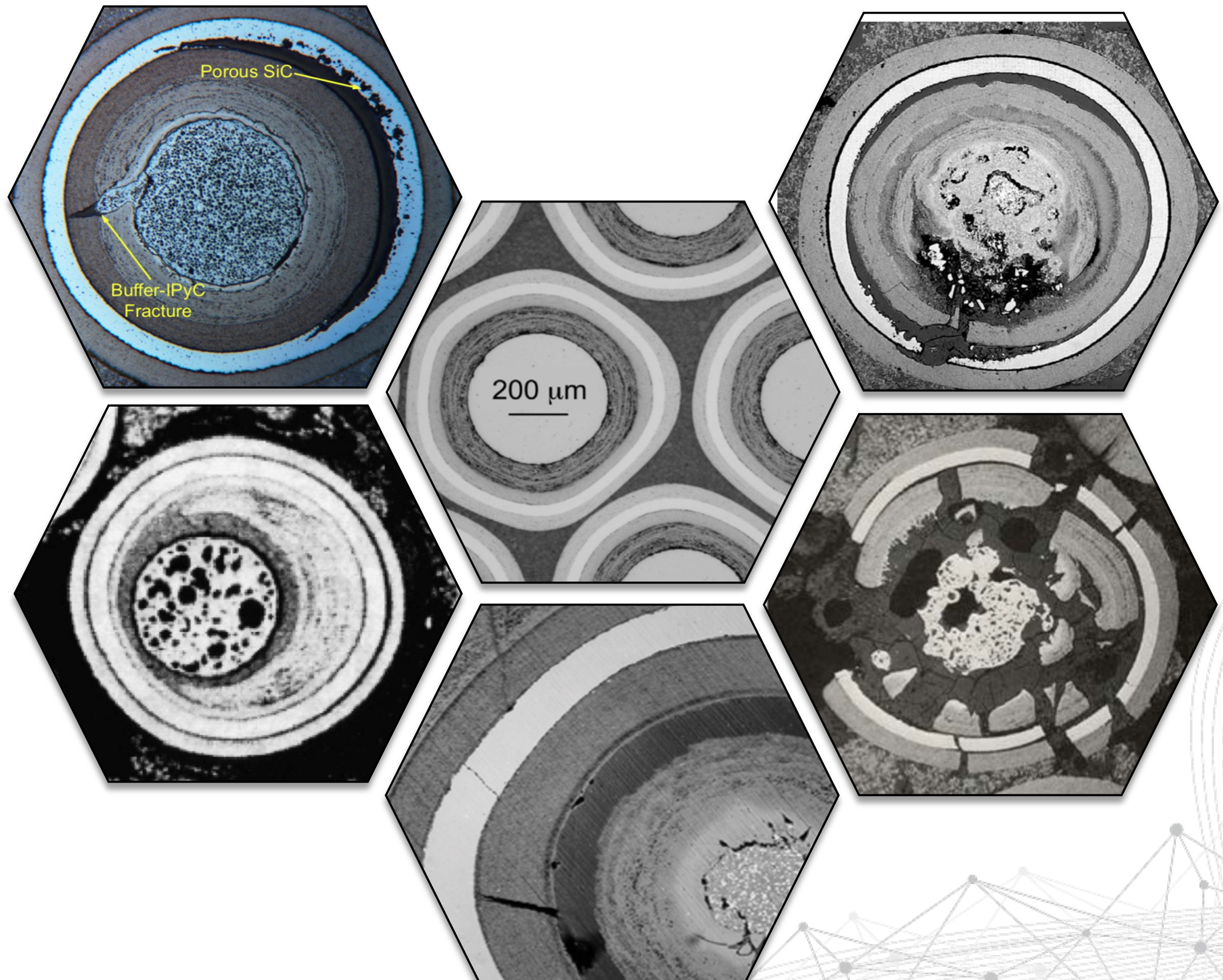


Tangential stress in SiC

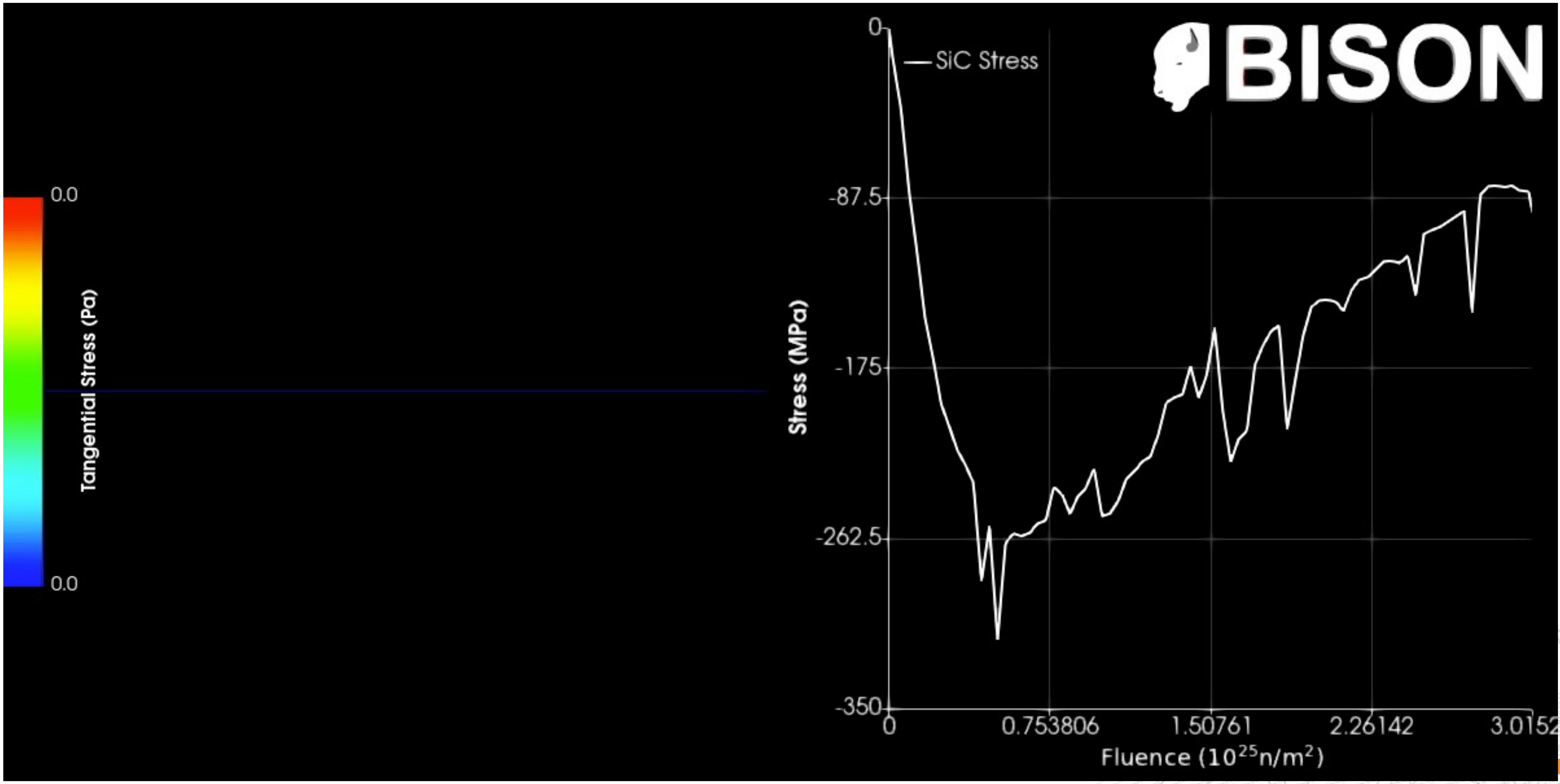
TRISO Failure Modes

- **Mechanical**
  - Pressure vessel failure
  - Irradiation-induced PyC failure leading to SiC cracking
  - IPyC-SiC / Buffer-IPyC partial debonding

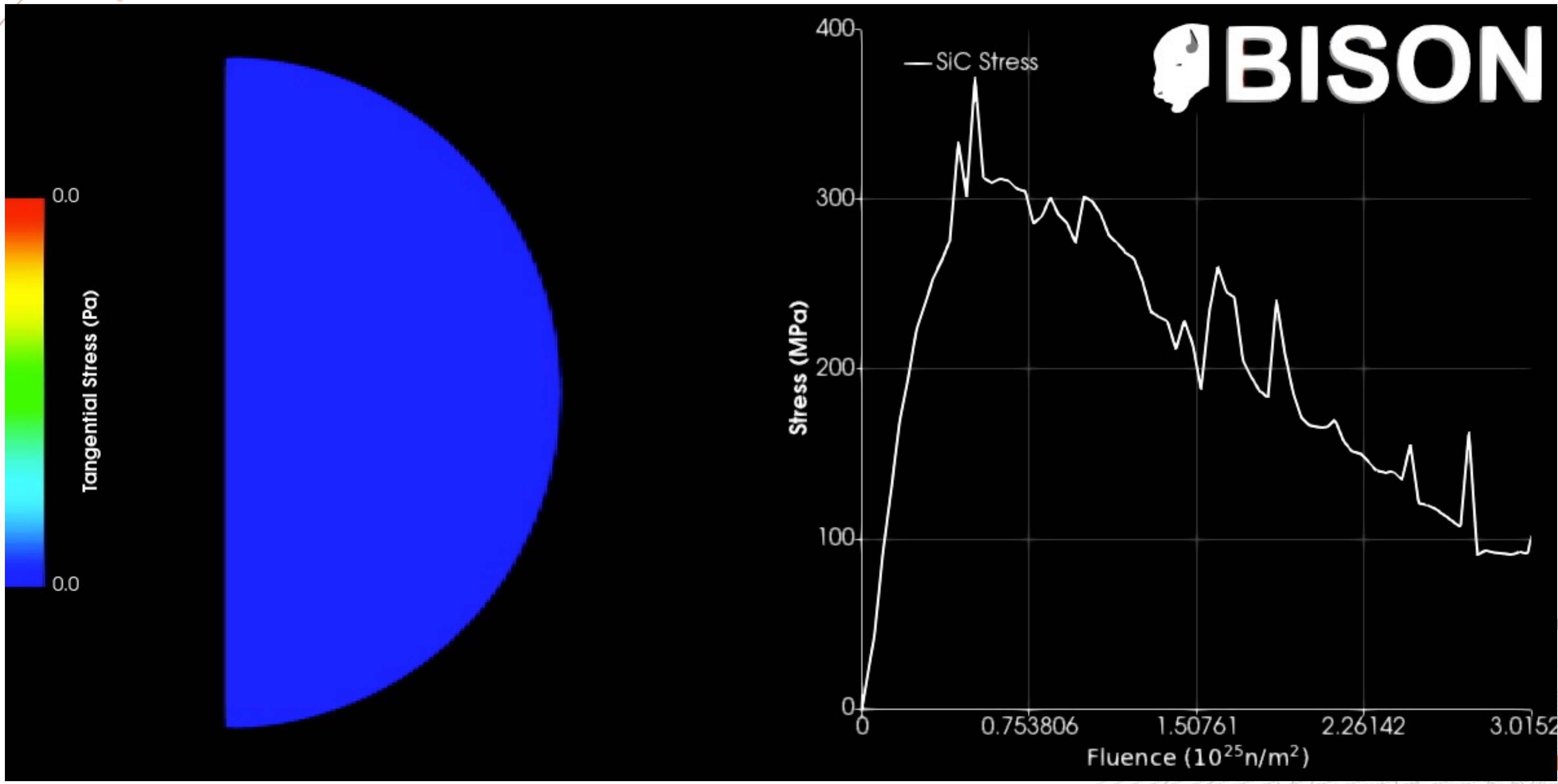
- **Thermochemical**
  - Kernel migration
  - SiC thermal decomposition
  - Fission product attack of SiC
  - Corrosion of SiC by CO



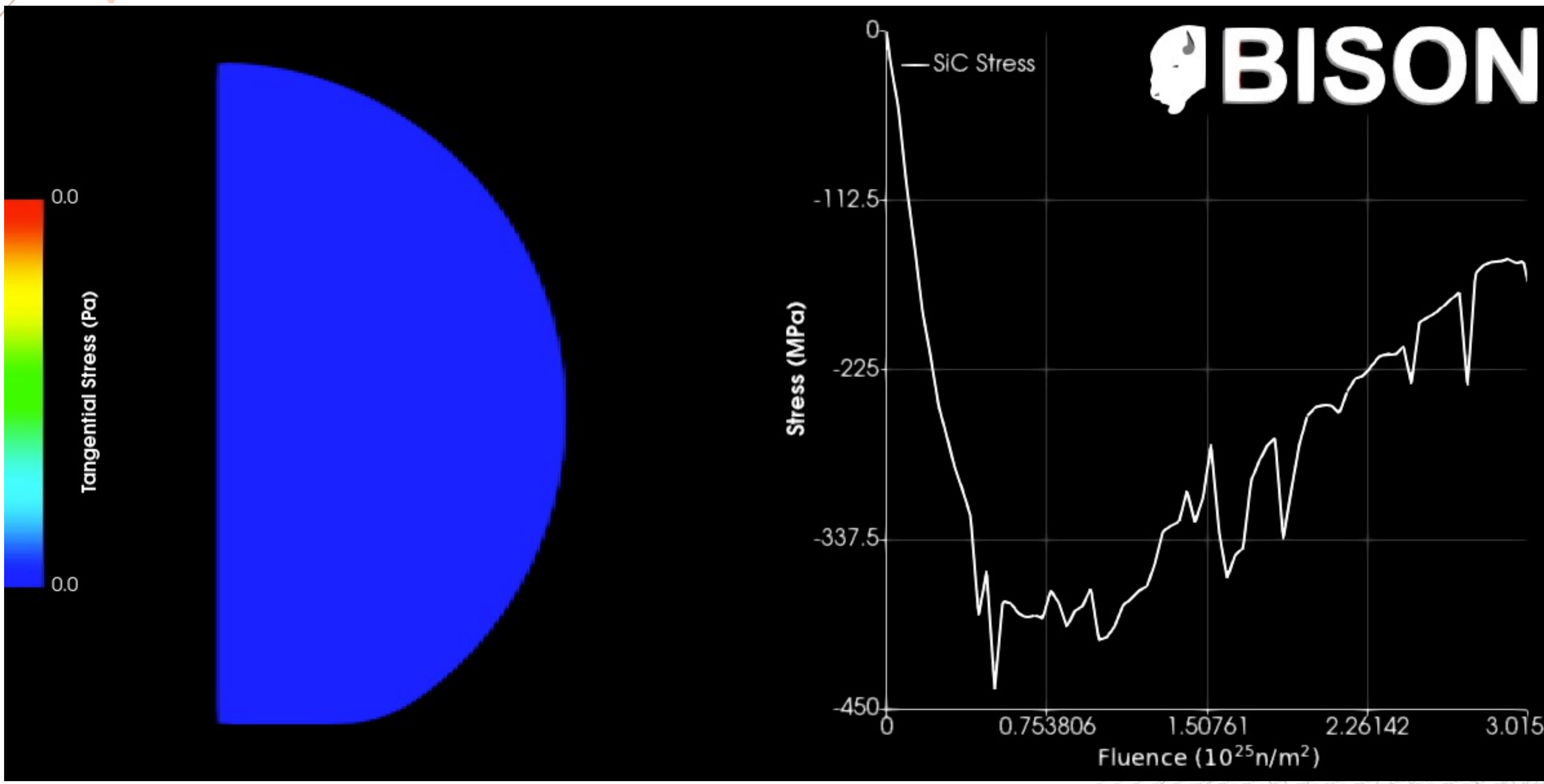
Pressure Vessel Failure



IPyC Cracking



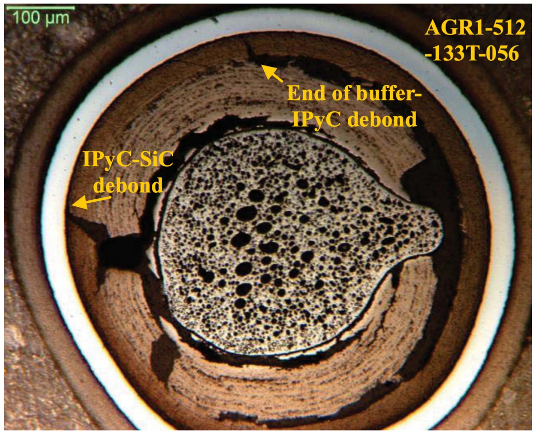
Aspherical Particle



Particle Debonding

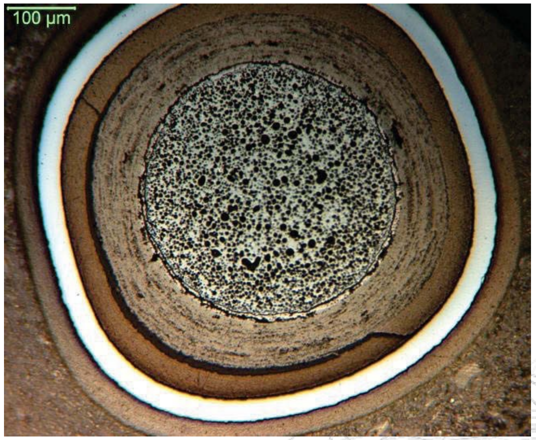
Partial debonding of the IPyC from the SiC

- ❑ Partial debonding between the IPyC and the SiC has also been observed in PIE of the NP-MHTGR fuel particles.
- ❑ During irradiation, shrinkage of the IPyC layer induces a radial tensile stress at the interface between the IPyC and SiC layer.
- ❑ If the stress exceeds the bond strength between layers, then debonding of the IPyC from the SiC occurs.
- ❑ A stress concentration occurs in the SiC layer at the tip of the debonded region, containing tensile stress components that could contribute to failure of the SiC.

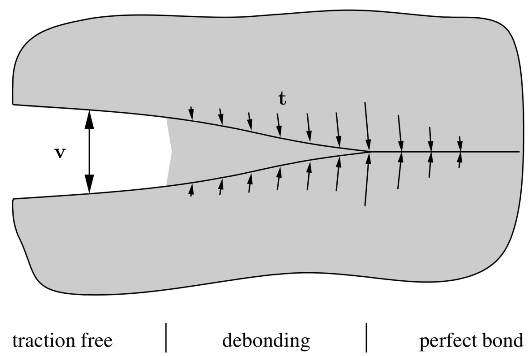


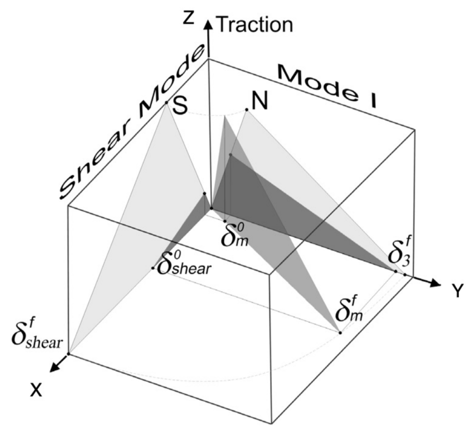
Buffer-IPyC partial debonding in AGR-1

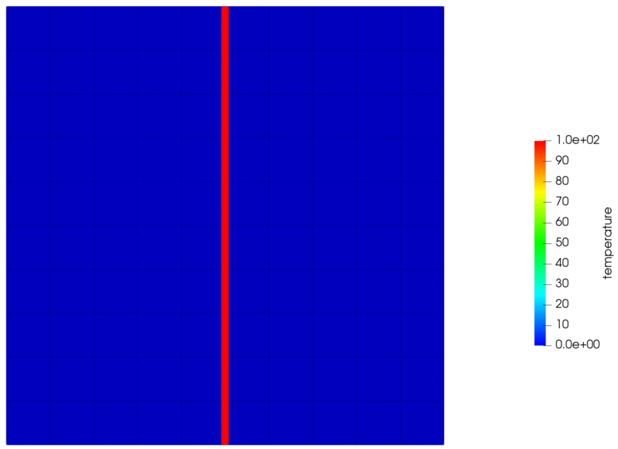
- ❑ Buffer-IPyC partial debonding were found with intermediate frequency in AGR-1 compacts and it can lead to IPyC cracking and separation from SiC layer.
- ❑ Allows localized attack of SiC layer by fission products (especially Pd)
- ❑ Pd attack can eventually result in loss of FP retention by SiC layer.
- ❑ Degradation is worse at higher safety test temperatures

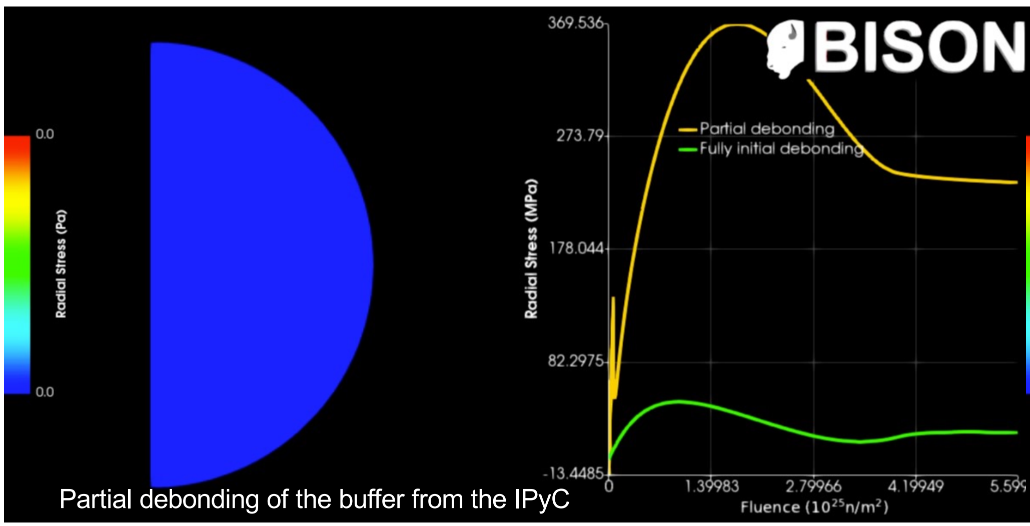


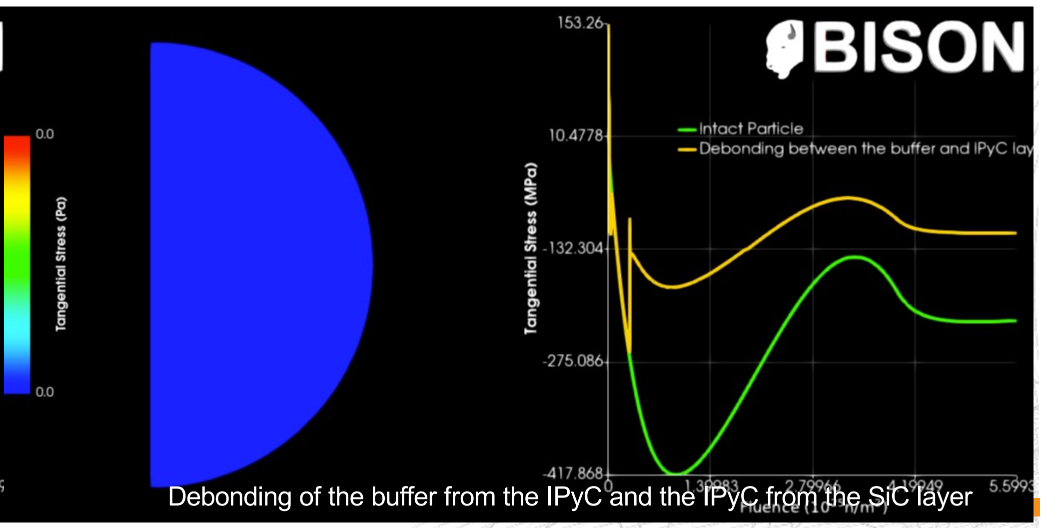
Debonding with Cohesive-zone Method











Weibull Failure Probability

- In the Weibull theory, the failure probability is:

$$P_f = 1 - \exp\left(-\int \left(\frac{\sigma_c}{\sigma_{ms}}\right)^m dV\right)$$

- A Weibull failure criterion is used to determine vessel failure for the PyC layer and SiC layer. The maximum stress σ_c is compared to a strength sampled from Weibull distribution. The failure probability is given as:

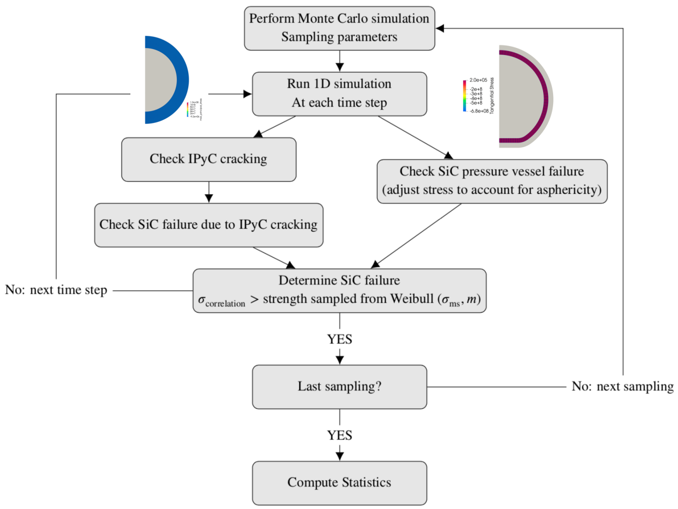
$$P_f = 1 - \exp\left(-\left(\frac{\sigma_c}{\sigma_{ms}}\right)^m\right)$$

- The effective mean strength σ_{ms} is given as

$$\sigma_{ms} = \frac{\sigma_0}{(In)^{1/m}}$$

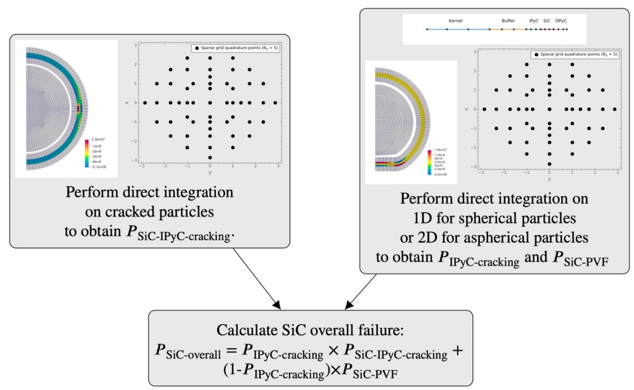
$$I_n = \frac{\int (\sigma_1{}^m + \sigma_2{}^m + \sigma_3{}^m)\, dV}{\sigma_c^m}$$

Statistical Approaches for Failure Analysis



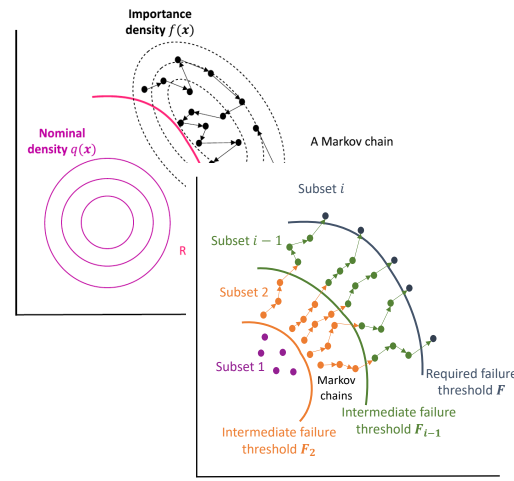
Classical Monte Carlo Approach:
- Most acceptable approach.
- Easy to expand for additional failure modes.
- Maximum 100 million samples with parallel computing on HPC.

W Jiang, Jason D. Hales, Benjamin W. Spencer, Blaise P. Collin, Andrew E. Slaughter, Stephen R. Novascone, Aysenur Toptan, Kyle A. Gamble, Russell Gardner, “TRISO Particle Fuel Performance and Failure Analysis with Bison”, Journal of Nuclear Materials, 548, 152795, 2021



Direct Integration Approach:
- Directly run 2D/3D TRISO simulation.
- Moderate computational cost: still much less than Monte Carlo simulation.

W Jiang, G. Singh, J.D. Hales, A. Toptan, B.W. Spencer, S.R. Novascone, S.L.N. Dhulipala, Z.M. Prince, “Efficient High-Fidelity TRISO Statistical Failure Analysis using Bison: Applications to AGR-2 Irradiation Testing”, Journal of Nuclear Materials, 153585, 2022.

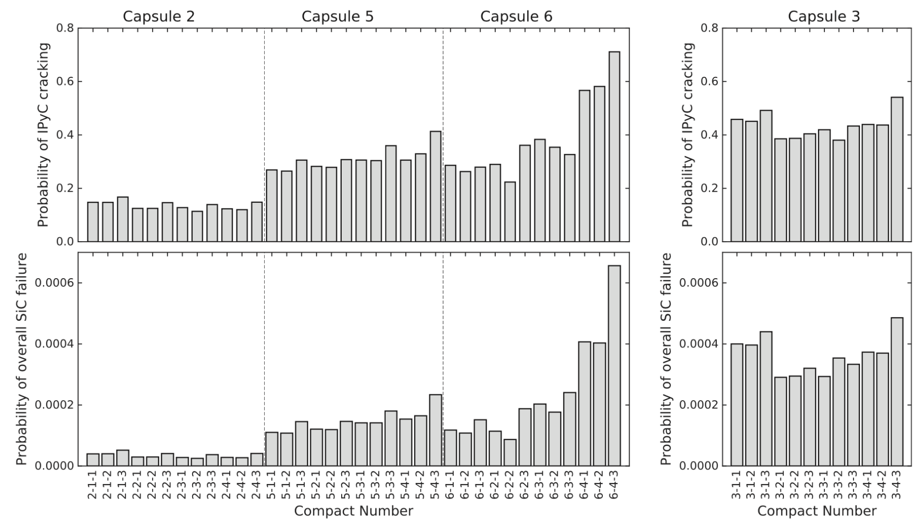


Variance Rduction Approach:
- Adaptive importance sampling and parallel subset simulation.
- Multifidelity TRISO failure modeling.
- Statistical failure characterization.

S.L.N. Dhulipala, W Jiang, B.W. Spencer, J.D.Hales, M.D.Shields, A.E.Slaughter, Z.M.Prince, V.M. Labour´e, C Bolisetti, P Chakroborty, “Accelerated Statistical Failure Analysis of Multifidelity TRISO Fuel Models”, Journal of Nuclear Materials, 153604, 2022

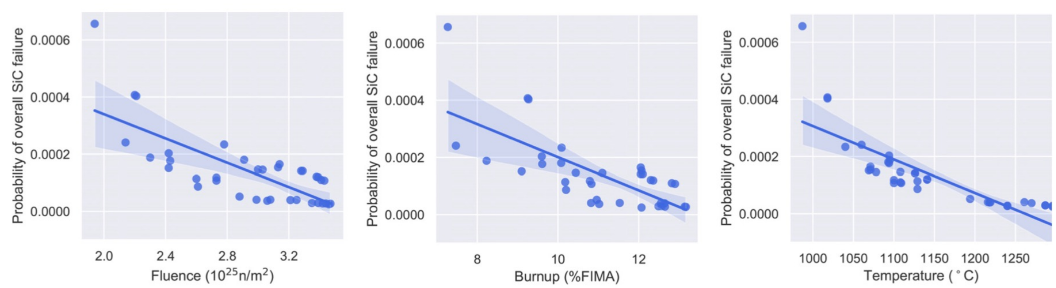
Failure Probability Calculation for AGR-2 Compacts

Category	Parameter	Fuel Type
		UCO
Fuel Characteristics	235U enrichment (wt%)	14.029
	Carbon/uranium (atomic ratio)	0.392
	Oxygen/uranium (atomic ratio)	1.428
Particle geometry	Kernel diameter (μm)	426.7±8.8
	Buffer thickness (μm)	98.9±8.4
	IPyC(μm)	40.4±2.5
	SiC thickness (μm)	35.2±1.2
	OPyC thickness (μm)	43.4±2.9
	Particle asphericity	1.037±0.011
Fuel properties	Kernel density (g/cm³)	10.966
	Buffer density(g/cm³)	1.05
	IPyC density(g/cm³)	1.89±0.0011
	OPyC density(g/cm³)	1.907±0.007
	IPyC BAF	1.0465±0.0049
	OPyC BAF	1.0429±0.0019



(a) UCO failure probability

(b) UO_2 failure probability



Fisson Product Diffusion

Conservation of fission product species:

$$\frac{\partial C}{\partial t} + \nabla \cdot \boldsymbol{J} + \lambda C - p = 0$$

Mass flux:

$$\boldsymbol{J} = -\mathrm{D}\nabla C$$

Diffusion Coeffient:

$$\mathrm{D} = \sum_i D_{0,i} \exp(\frac{-Q_i}{RT})$$

Mass passed outside the particle:

$$r = \int\int -D\nabla C \cdot n \, dt \, dA$$

Total fission product production:

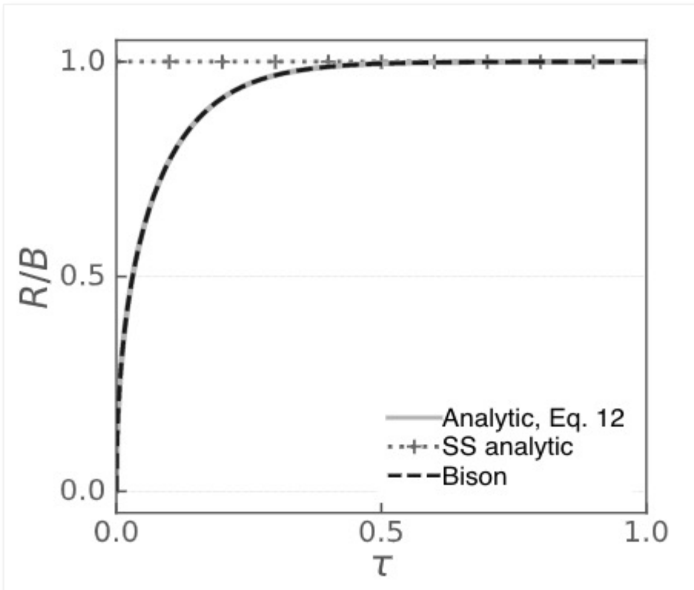
$$p = \int\int \Gamma \dot{F} \, dt \, dV$$

Release fraction:

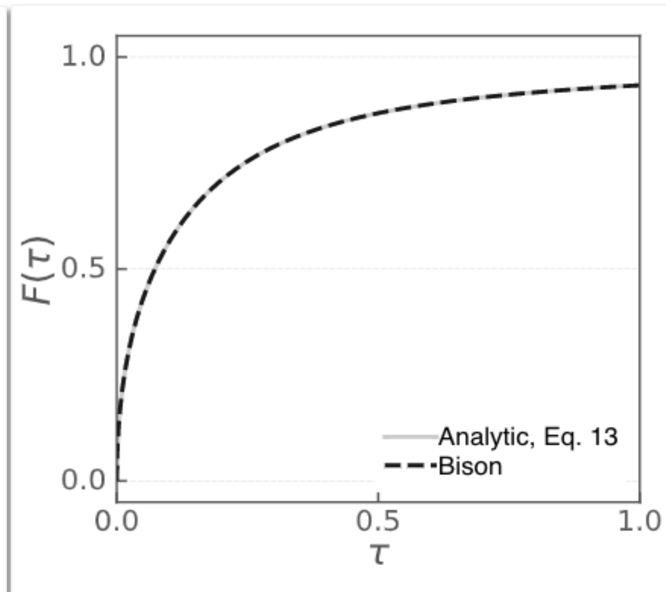
$$f = \frac{r}{p}$$

Verification problems:

- In-pile condition for a short-lived FP
- In-pile condition for a long-lived FP
- Out-of-pile condition
- Evaporation from the outer surface, for both short- and long-lived FPs

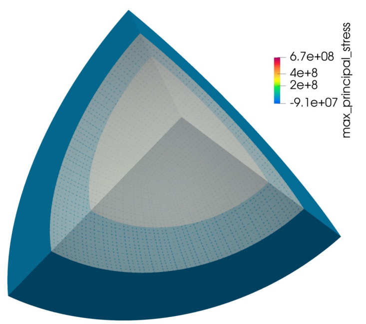


Release rate over birth-rate (R/B)

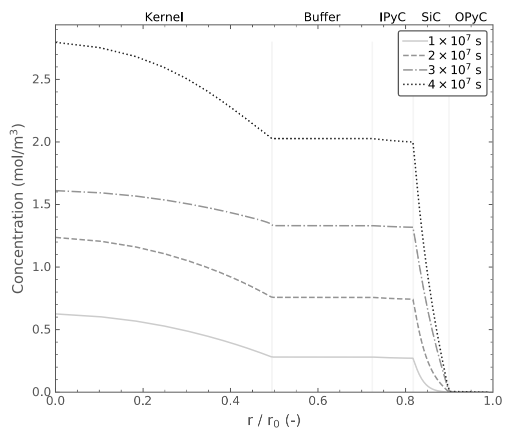


Release fraction

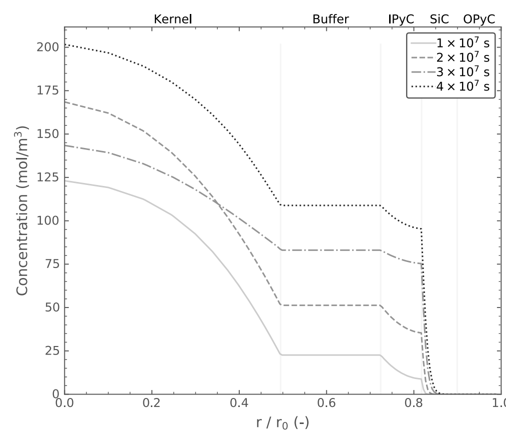
Fisson Product Diffusion Through Intact and Failed Particle



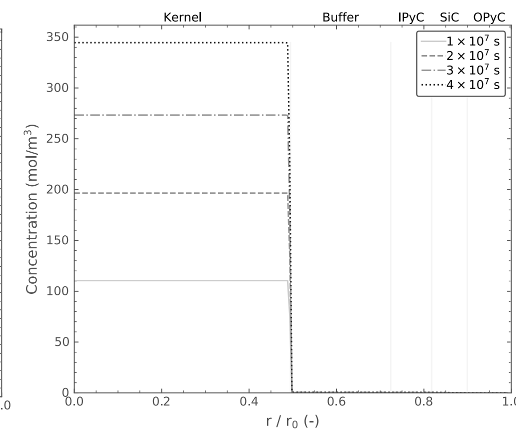
Intact Particle



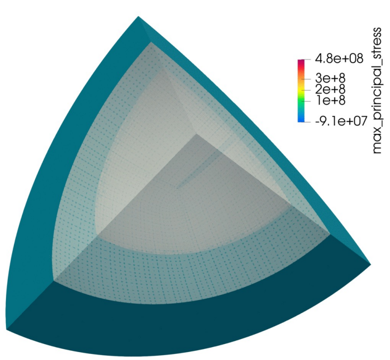
Silver



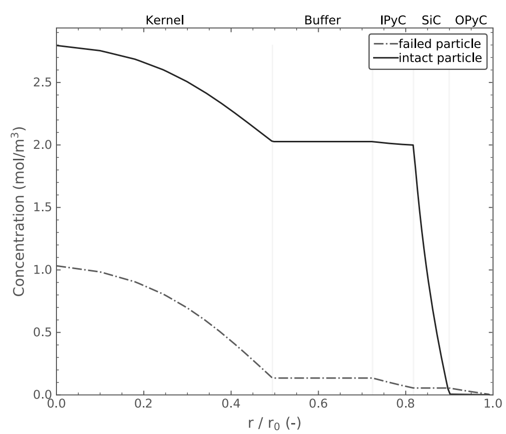
Cesium



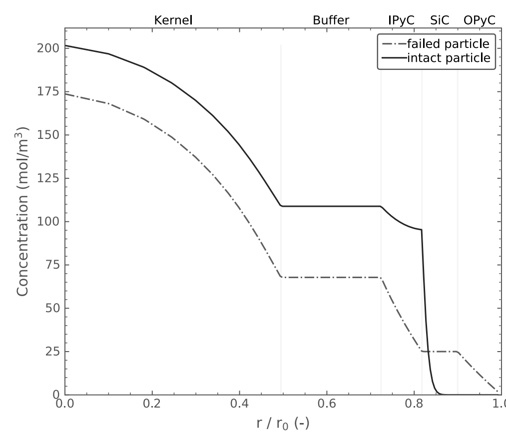
Strontium



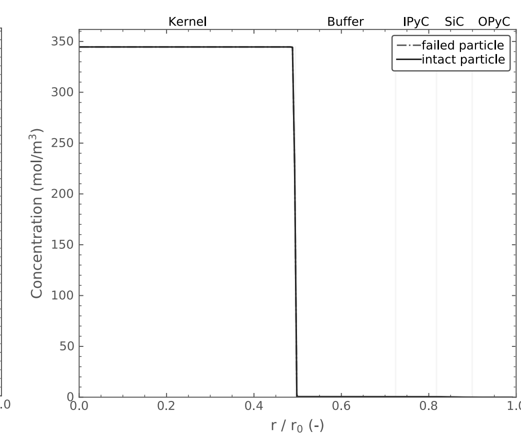
Failed Particle



Silver

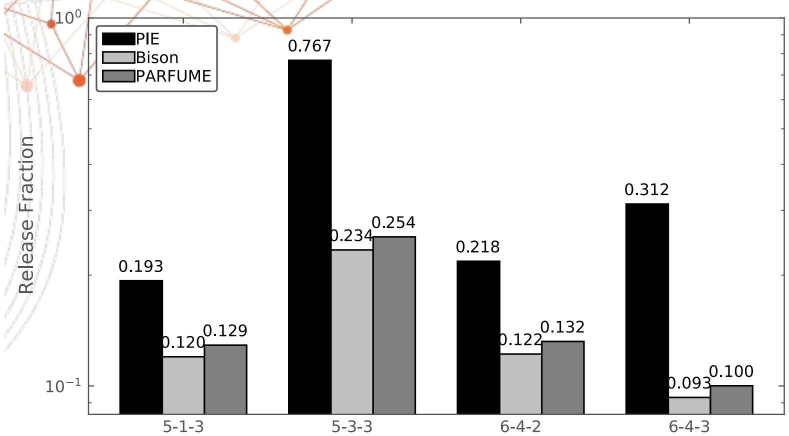


Cesium

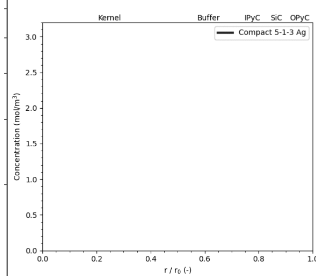


Strontium

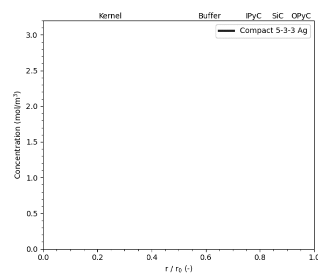
AGR-2 Validation



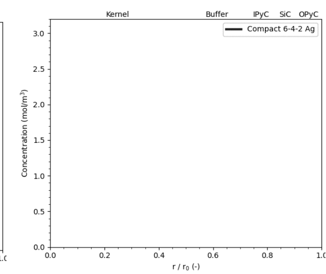
Silver release fractions



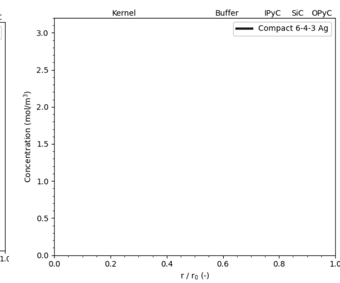
Silver compact 5-1-3



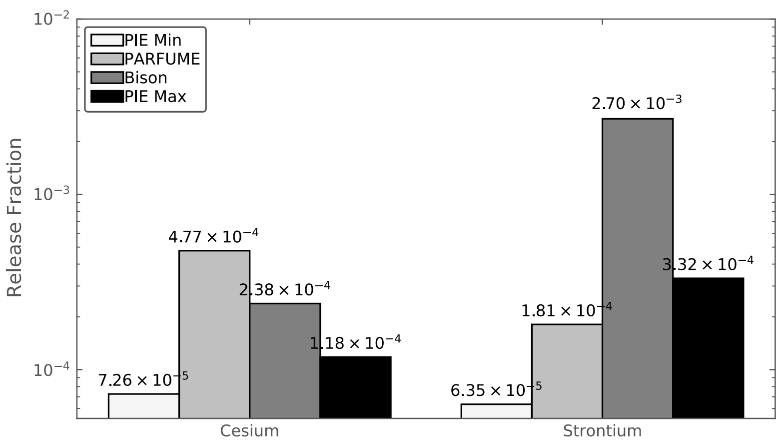
Silver compact 5-3-3



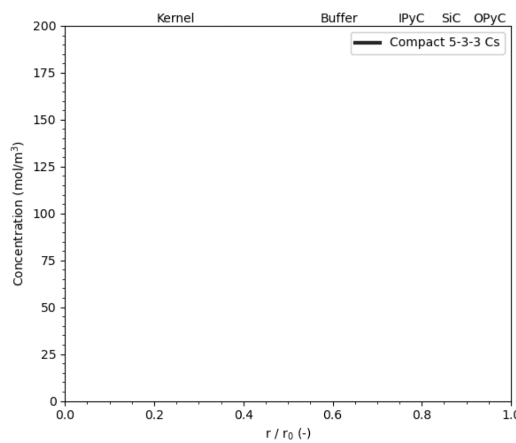
Silver compact 6-4-2



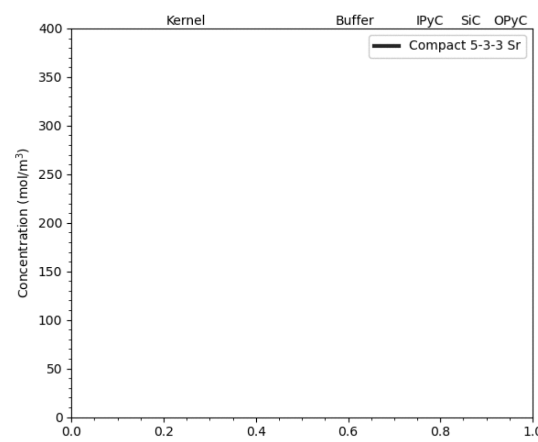
Silver compact 6-4-3



Cesium and Strontium release fractions (Compact 5-3-3)

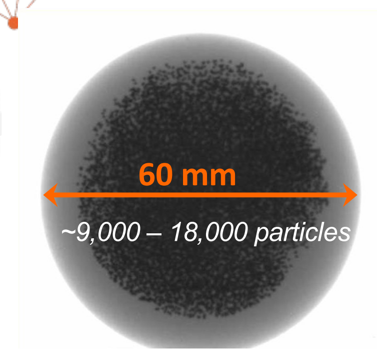


Cesium compact 5-3-3

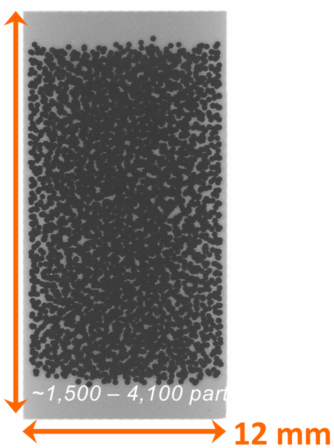


Strontium compact 5-3-3

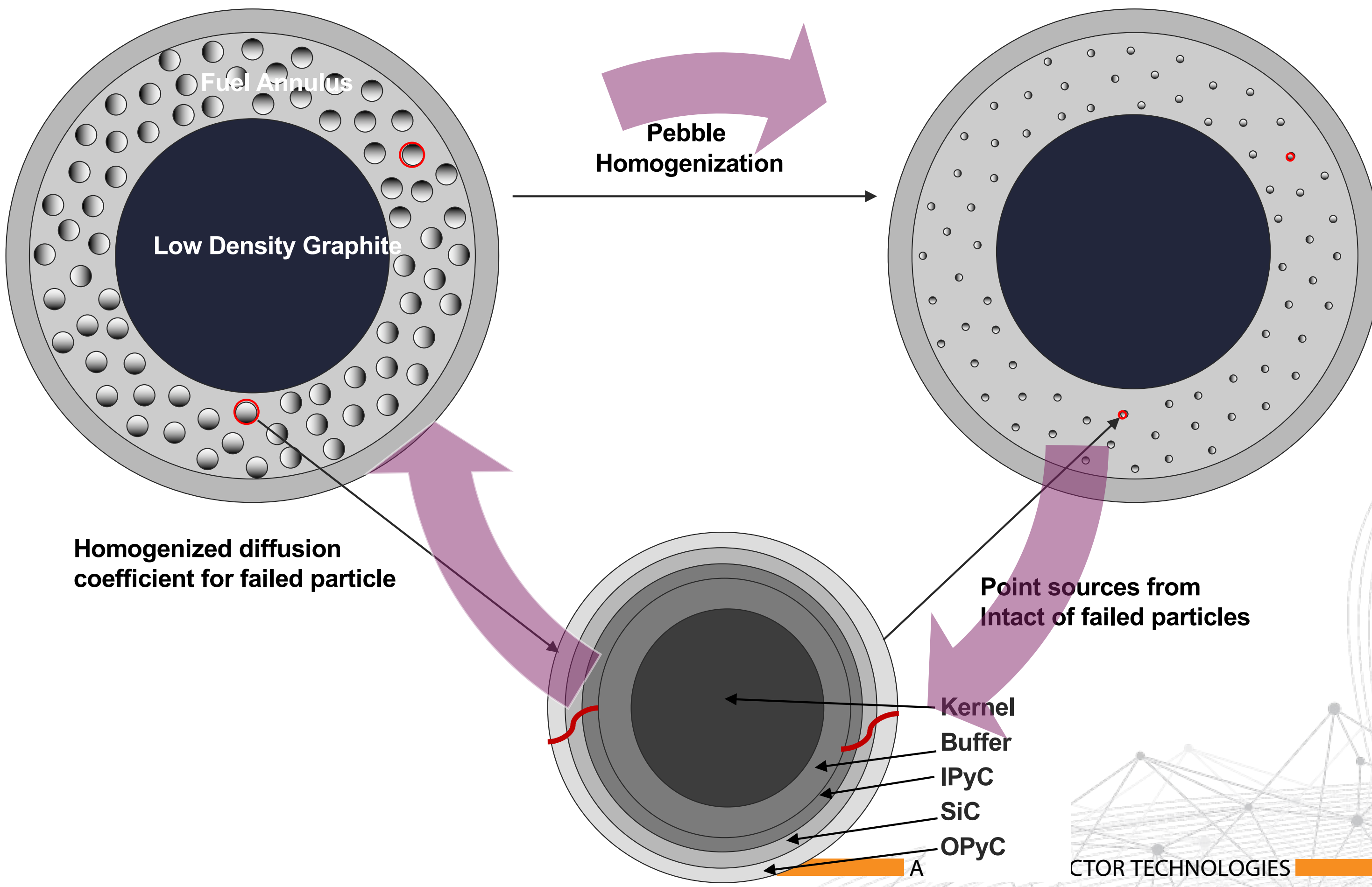
Fuel Elements Modeling



Spherical fuel elements

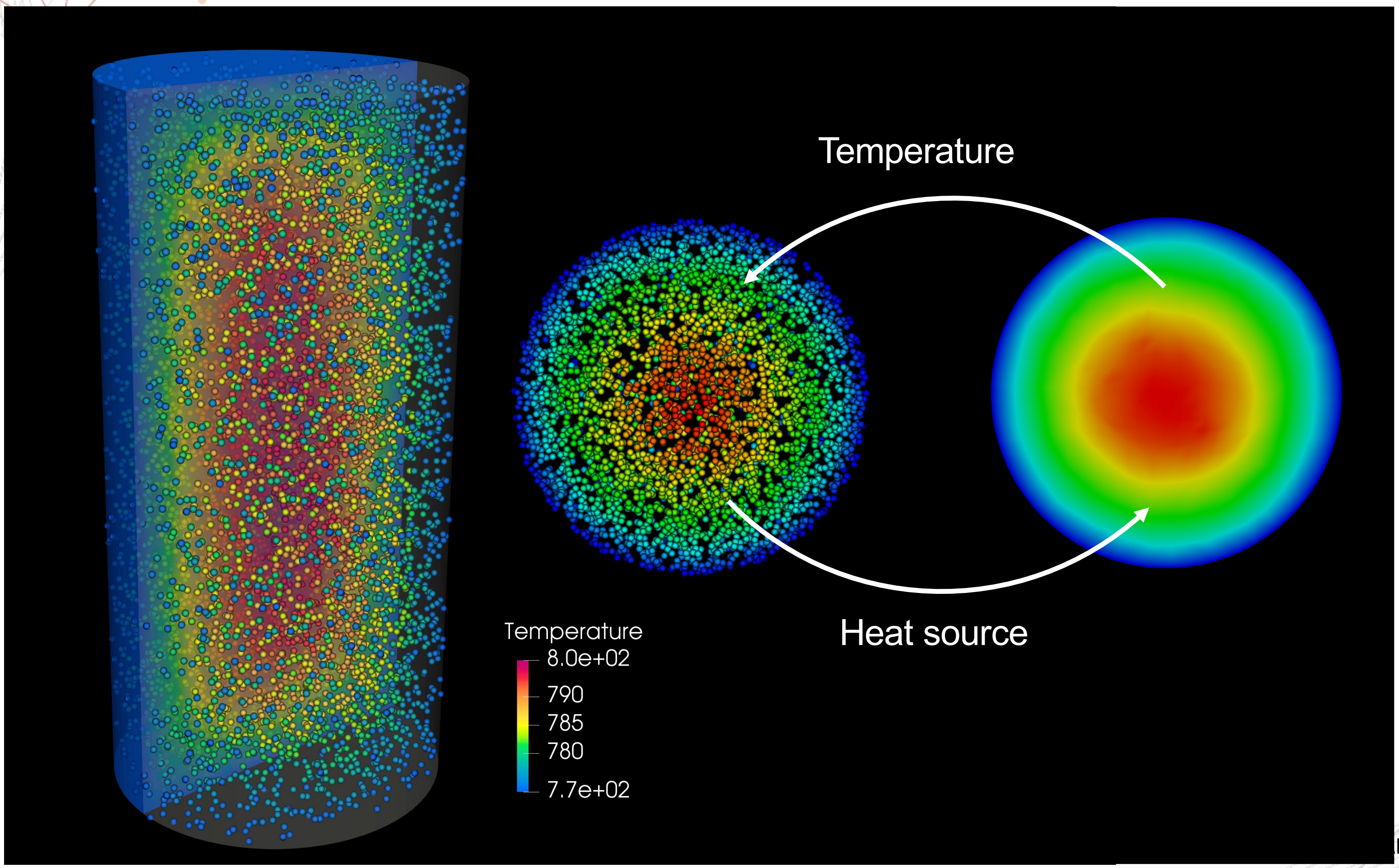


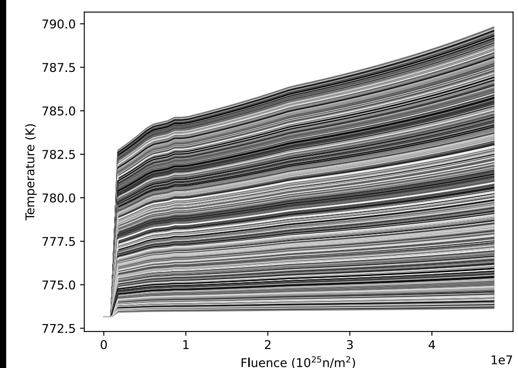
Cylindrical fuel elements



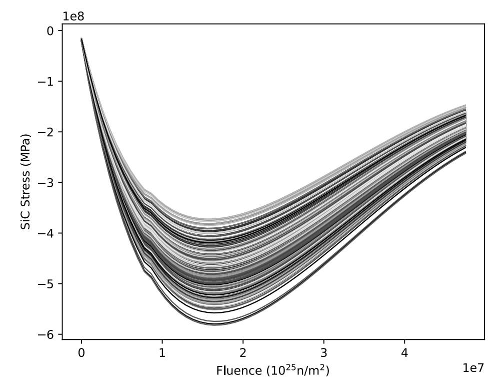
CTOR TECHNOLOGIES

Two-ways Coupling Between Particles and Matrix





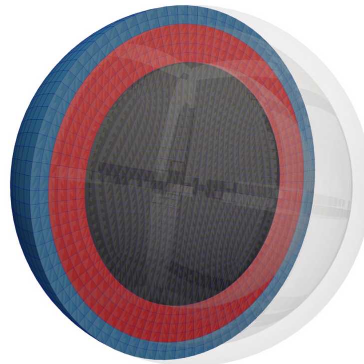
Exterior temp of all particles

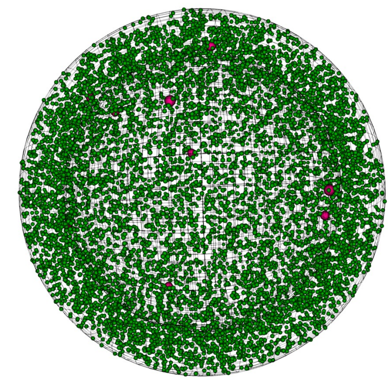


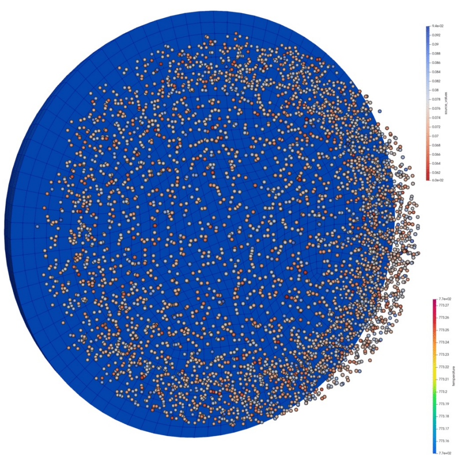
SiC stress of all particles

Pebble Modeling

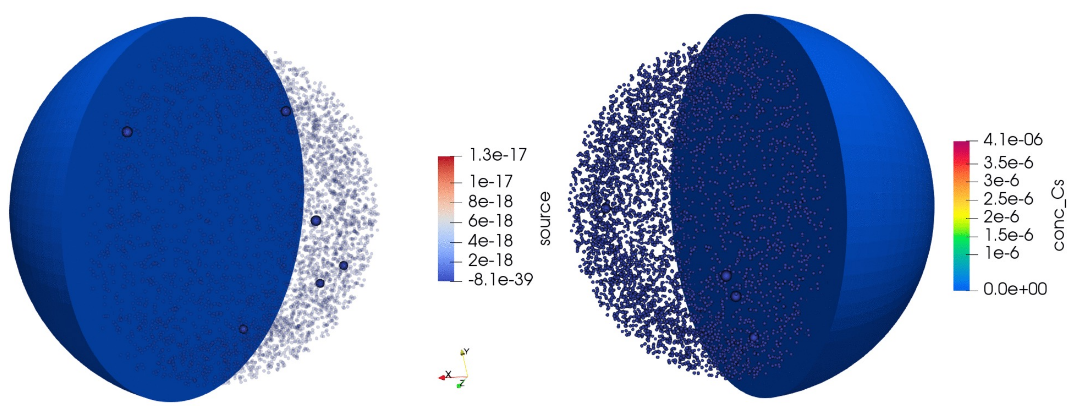
RADIUS (CM)	2.000
SHELL LAYER THICKNESS (CM)	0.200
FUEL LAYER THICKNESS (CM)	0.420
(AGR-5/6/7) TRISOS	9022
U-235 ENRICHMENT (% WT)	19.55



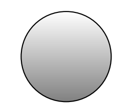




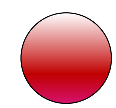
Heat point source



Cs point source



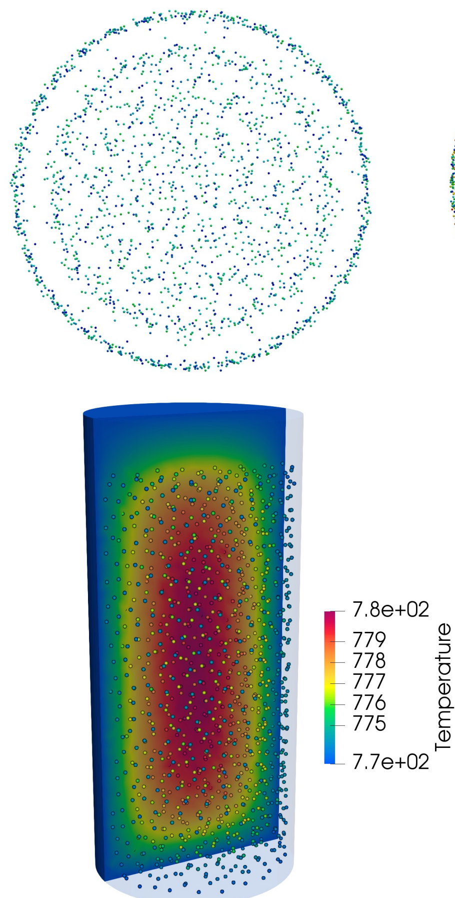
9012 intact particles



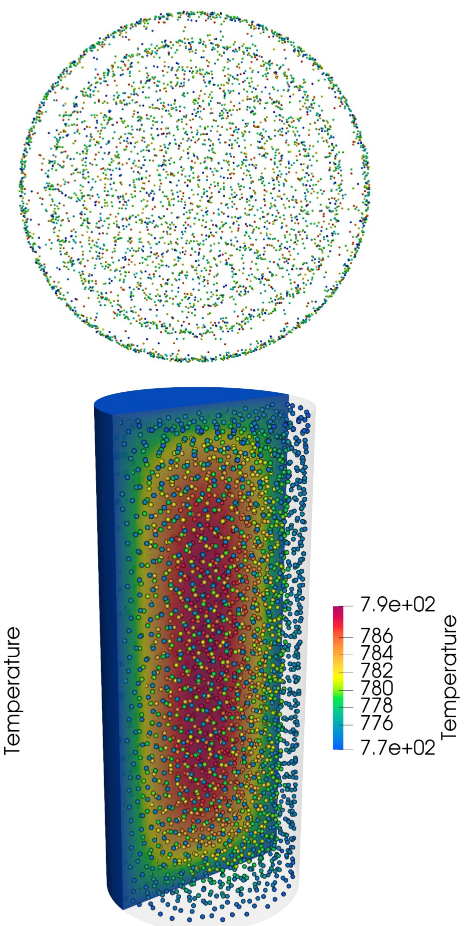
10 failed particles

AGR Compacts

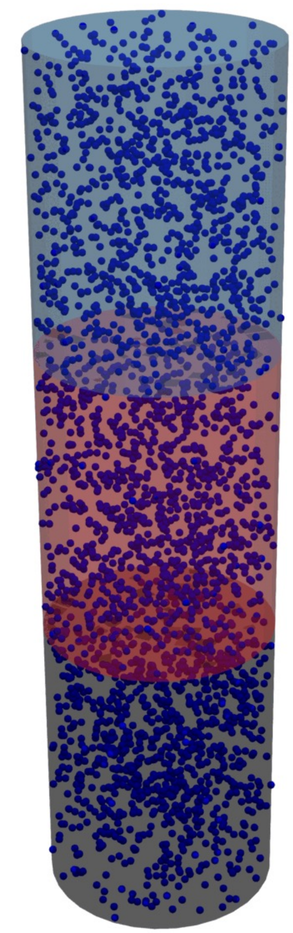
X-ray microscope of TRISO kernel



25% PF

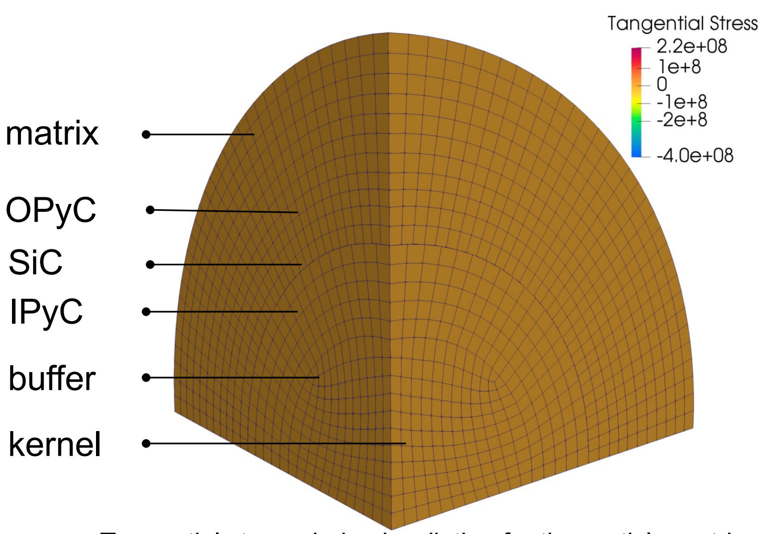


48% PF

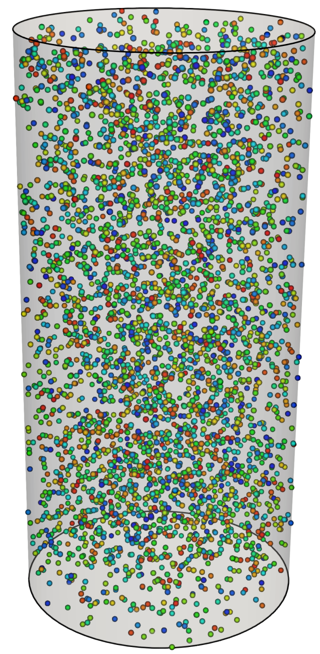


Graphite Matrix Modeling

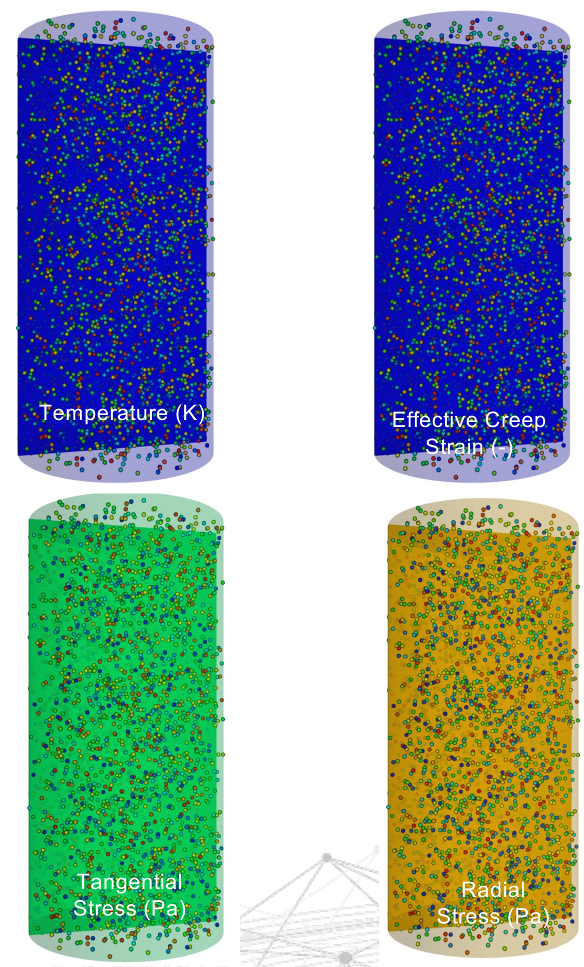
- **The cores and reflectors in HTGRs are made of graphite materials**
  - the graphite acting as a moderator, a fuel host matrix, a structural component to provide
    - channels for fuel, coolant gas, and control rods
    - a thermal/neutron shielding component
    - heat sink/conduction path during transients



Tangential stress during irradiation for the particle-matrix debonding example (displacements are magnified 2x)



Fuel compact containing 4,000 TRISO particles randomly generated from an MC simulation.



AGR-3/4

- AGR-3/4 is the combined third and fourth planned irradiations of the AGR Fuel Development and Qualification Program
- Irradiate fuel containing uranium oxycarbide (UCO) designed-to-fail (DTF) fuel particles that will provide a known source of fission products for subsequent transport through compact matrix and structural graphite materials.