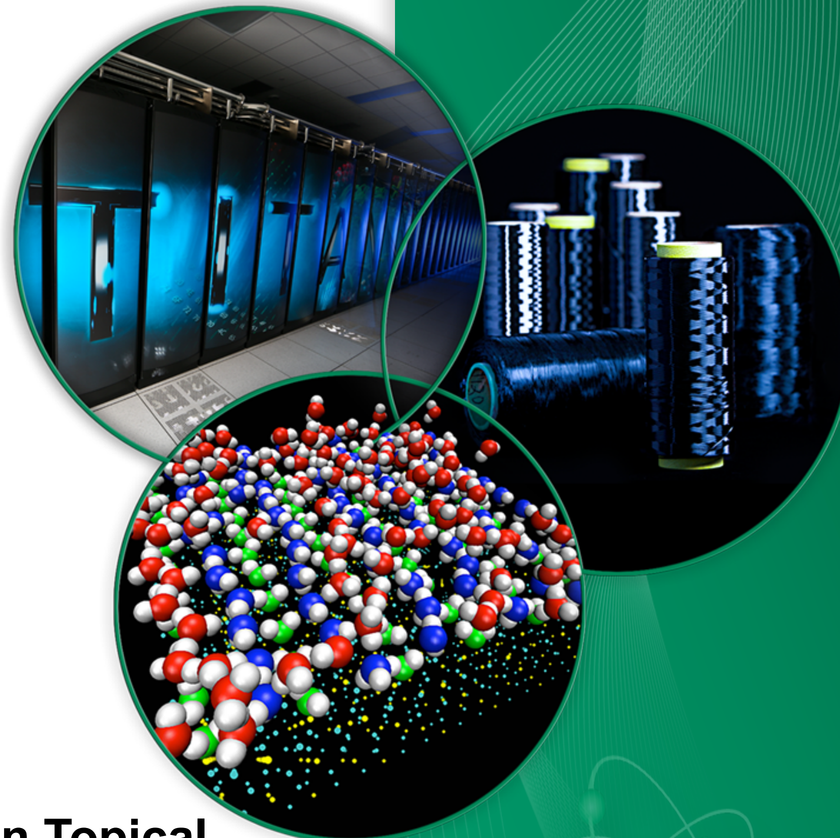
Enhancements in Continuous-Energy Monte Carlo Capabilities in SCALE



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Outline

- Enhancements in CE Data and Transport
- New KENO Features
- New SCALE CE Monte Carlo (MC) Sequences
- CE efficiency Improvements
- Summary

Enhancements in CE Data

AMPX processes ENDF-formatted nuclear data evaluations to provide continuous energy (CE), multi group (MG) and covariance data libraries to SCALE.

Released SCALE CE data libraries:

- Only provide CE neutron data library with a few reactions
- Some biases observed/reported (with SCALE 6.1)
  - for thermal system ← S(α,β) data
  - for intermediate energy range ← probability tables that provide CE treatment in the unresolved resonance range

Enhancements in CE Data

New SCALE CE data libraries:

- Neutron data library:
  - Improvements in probability tables, S(α,β) data, 2D collision kinematics, etc ➔ significant reduction in bias in the results
  - Have been extended to support a wide range of reactions
- Gamma data library:
  - Have the same format as the neutron libraries
  - Coherent scattering, incoherent scattering, pair production, and photoelectric absorption reactions are included in the libraries for each element
  - Photoelectric absorption is treated as a terminal process (no secondary particles)
- Gamma yields:
  - Provide gamma yield data from CE neutron interactions for coupled neutron-photon particle transport

All libraries will be available with SCALE6.2 (ENDF-B/VII.1)

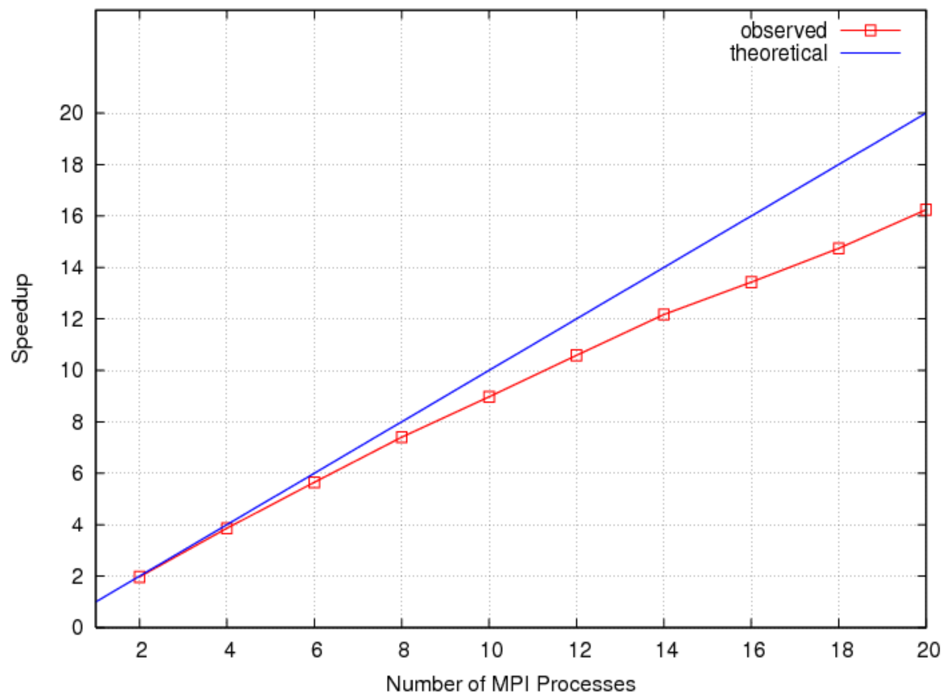
Enhancements in CE transport

- A new CE physics engine, SCEMPP (Scale CE Modular Physics Package) was designed to support all MC transport codes in SCALE
  - Fortran and C++ APIs to support both legacy and future developments
  - Models particle collisions in a material and generates the particle(s) resulting from a collision
  - Also provides non-transport data, such as reaction responses and point detector data
  - Integrated to the Monaco code and MAVRIC sequence to provide CE particle transport for shielding and CAAS analyses (CE-Monaco/MAVRIC)
  - Will be integrated in KENO after adding fission treatment

New KENO Features (available in SCALE 6.2):

Parallel KENO

- KENO joined parallel MC codes family
- Simple master-slave approach via MPI
- Domain replication
- Reproducible results
- Updating fission banks and tallies at the end of each generation
- Communication overhead due to these frequent updates



Parallel speed up of KENO-VI code in a depletion calculation.

- Parallel performance is strongly dependent on problem size and parameters
- Good scaling observed in CASL reference solution calculations with CE KENO (120-384 MPI processes)

New KENO Features (available in SCALE 6.2):

Multiple Mesh Support

- Previous KENO versions support only one mesh with a single mesh-based quantity
- This new feature enables multiple mesh definitions for tallying several mesh-based quantities

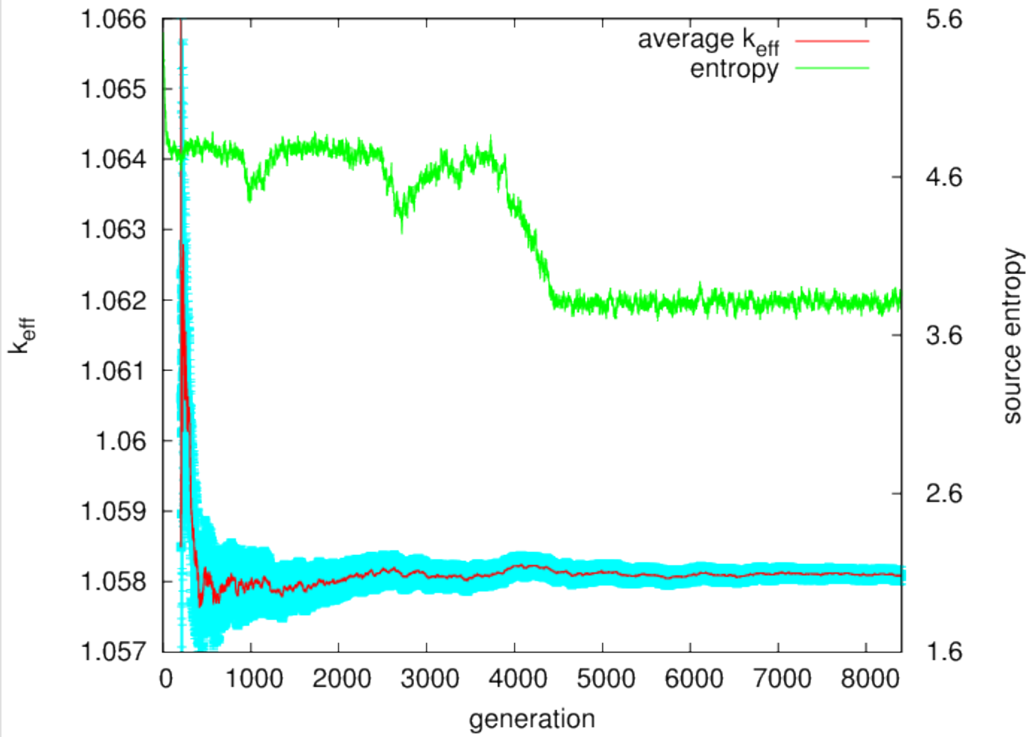
➔Enables:

- Mesh-based Source Convergence Diagnostics
- CE-TSUNAMI F*(r) mesh
- Mesh-based fission matrix approach
- Fission source tally (CADIS)
- Mesh fluxes
- …

New KENO Features (available in SCALE 6.2):

Source Convergence Diagnostics

- Relies on Shannon Entropy statistics[1,2,3]
- Accumulates fission source at each generation on a user-defined Cartesian mesh (default mesh size 5x5x5, covers entire geometry)
- Post-processes the accumulated fission source and computes entropy, relative entropy, average entropy, etc for three tests:
  - Test-1: Final Convergence
  - Test-2: First Converged Generation
  - Test-3: Adequate Active Generation



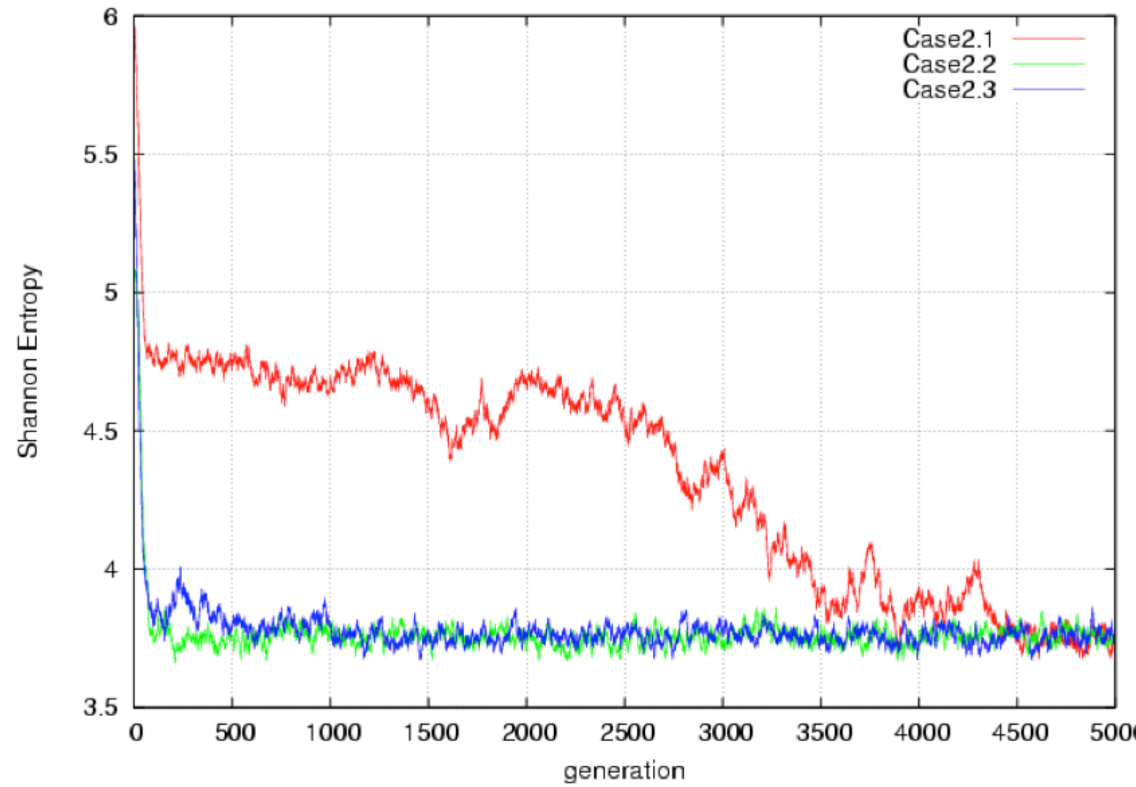
1. T. Ueki and Forrest B. Brown, **“**Stationarity and Source Convergence Diagnostics in Monte Carlo Criticality Calculation,” Nuclear Mathematical and Computational Sciences Conference (M&C 2003), Gatlinburg, Tenn., April 6–10, 2003.
2. T. Ueki and F. B. Brown, “Stationary Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations,” *Nuclear Science & Engineering* **149**, 38 (2005).
3. M. Wenner and A. Haghighat, “Study of Methods of Stationarity Detection for Monte Carlo Criticality Analysis with KENOV.a,” *Trans. Am. Nucl. Soc.*, ***97***, 647–651 (2007).

New KENO Features (available in SCALE 6.2):

Source Convergence Diagnostics

A benchmark problem from OECD NEA WPNCS Expert Group on Source Convergence

Case-2.2 and Case-2.3 easily converge, but Case-2.1 requires many generations skipped for convergence



Model	Test 1 (Final Convergence)	Test 2 (First Converged Generation)	Test3 (Adequate Active Generation)
Case 2.1	Passed	Failed (4,581)	Passed
Case 2.2	Passed	Failed (4)	Passed
Case 2.3	Passed	Failed (552)	Passed

New KENO Features (available in SCALE 6.2):

On-the-fly mixture total and absorption cross-section calculations

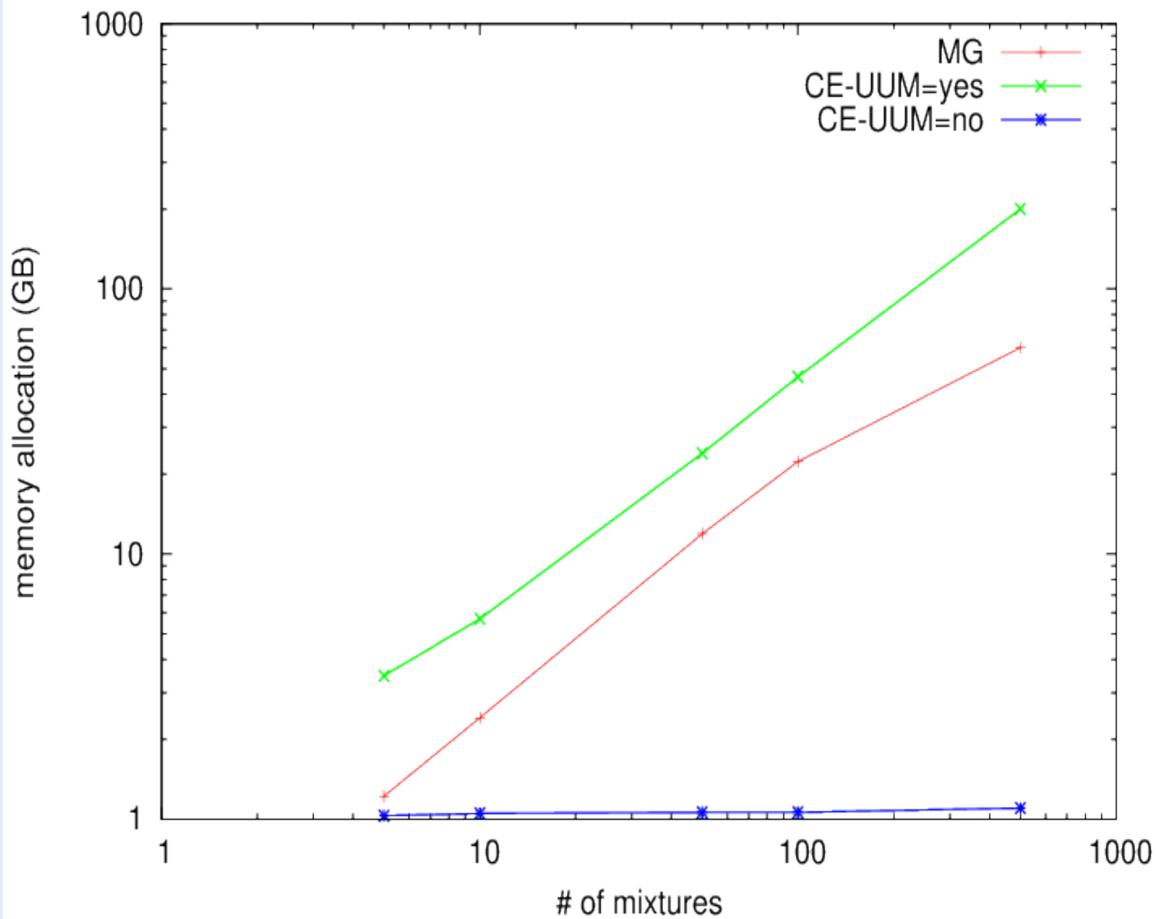
- CE calculations in KENO through SCALE 6.1 uses "unionized energy grid," where material-dependent cross-section data are generated and stored for each user-defined mixture
  - Memory allocation increases with the number of mixtures
- Alternative approach: on-request mixture cross-section calculation
  - Memory requirement is almost independent from the number of mixtures in the model
  - Up to 40 % additional computational overhead → but makes CE-TRITON, CE-TSUNAMI, CSAS6 calculations viable for the models with several mixtures

New KENO Features (available in SCALE 6.2):

➔ CE-UUM=yes refers the CE transport with unionized energy grid model

➔ CE-UUM=no refers CE transport with on-the-fly mixture cross-section calculations

➔ Memory allocation for MG KENO-VI calculation also includes the memory requirement of cross-section processing tools



MG & CE-UUM=yes requires >> 60 GB memory for the model with 500 mixtures

New KENO Features (available in SCALE 6.2):

Few-group microscopic reaction cross-section calculations

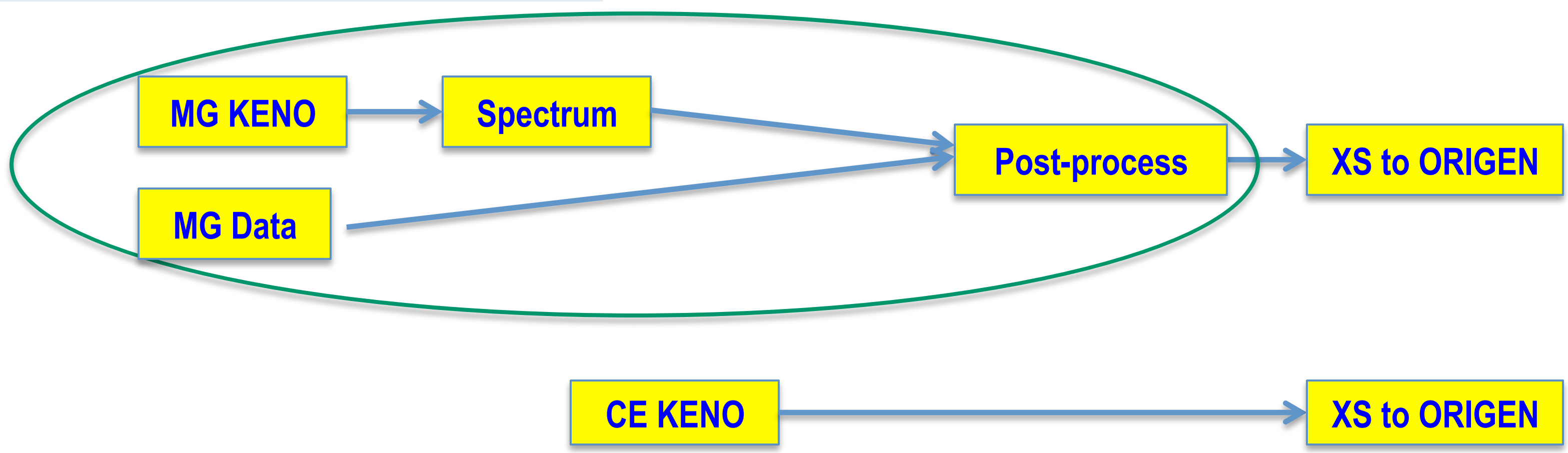
- For all/selected mixtures in the model
- Uses track-length estimator for reaction rate tallies
- Uses track-length estimator for fluxes
- Uses reaction rate tallies and fluxes to compute microscopic reaction cross-sections
- User can specify energy group structure for tallying(Default 238 groups)

➔ enables: **CE-TRITON**

(new CE depletion module)

TRITON (MG):

CE-TRITON:



New KENO Features (available in SCALE 6.2):

Doppler Broadening Rejection Correction Method (DBRC)

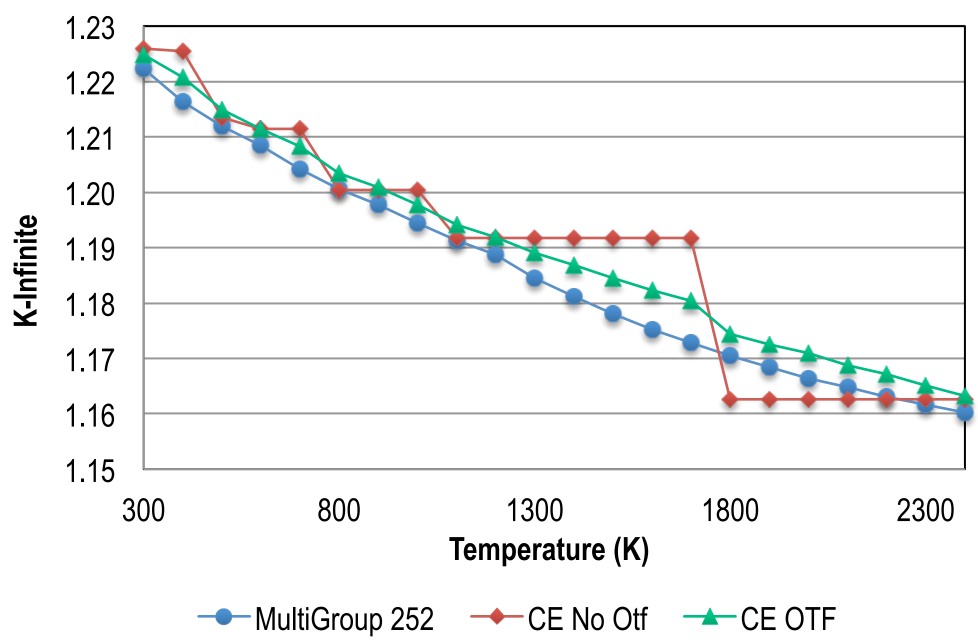
- Thermal motion of target nuclides can significantly affect the collision between a neutron and nucleus in the epithermal energy range
- CE KENO uses free-gas scattering model to simulate this thermal motion
- DBRC method introduces corrections to the Doppler broadening of the scattering kernel with a new sampling equation
- Implementing this method can have significant impact on eigenvalue calculations due to the increase of neutrons being upscattered into absorption resonances
- Temperature increases ➔ more neutrons upscattered into the resonances, resulting in more absorptions and a lower eigenvalue (*keff*)
- Especially significant in reactor applications rather than criticality safety

Temperature (K)	CE KENO	CE KENO with DBRC	Difference (pcm)
293.6	1.34460	1.34451	-9
600.0	1.33053	1.32932	-121
900.0	1.31759	1.31759	-182
1200.0	1.31029	1.30730	-299
1400.0	1.28113	1.27478	-635

New KENO Features (available in SCALE 6.2):

Cross-section Temperature Correction (pre-broadening)

- Libraries contain cross-section data typically broadened to a few temperatures
- If temperatures in the model are different than those present in the library ➔
  - MG KENO allows temperature correction through linear interpolation
  - CE KENO uses the closest temperature ➔ ~ a few hundred pcm differences



- 1D cross sections corrected using a finite difference method
  - Can pre-broaden cross sections before transport calculation
  - The same methodology can be used for true on-the-fly Doppler Broadening
- Planning to extend for the probability tables for unresolved resonance range
- Planning to determine ways to pre-broaden S(α,β) data

New SCALE Sequences with CE Transport

- CE-Monaco/MAVRIC with SCEMPP → criticality accident alarm system analyses
- CE-TRITON with CE-KENO → reactor analysis
- CE-TSUNAMI with CE-KENO → sensitivity & uncertainty

CE Performance Improvements

Observations/Issues:

- CE neutron data for KENO through SCALE 6.1 requires ~ 11.4 GB physical memory if all nuclides in the library are loaded (+430 nuclides)
- Size of CE data and additional memory requirement due to the newly added features limit both the serial and parallel KENO code performance

Memory footprint of CE data in CE transport has been reduced significantly by redesigning our codes and data!!!

Action	% Reduction in memory allocation
Changed format of internal data storage arrays (DBL-to-SNGL conversion)	15-45
Revisited 2D collision kinematics data and redesigned data containers for this data	5-30
Optimized nuclide object (data container)	3-15
TOTAL	20-90

Summary

- Significant improvements in CE Monte Carlo Capabilities of SCALE
  - New CE data with wide range of reaction, small memory footprint
  - New CE MC transport module, SCEMPP, for both legacy code and future developments
- CE KENO with new features enables more reliable calculations
  - Parallel KENO
  - Source Convergence Diagnostics
  - On-the-fly (on-request) mixture cross-section calculations
  - DBRC, pre-broadening, on-the-fly Doppler Broadening
  - …
- New CE sequences extend the range of SCALE applications