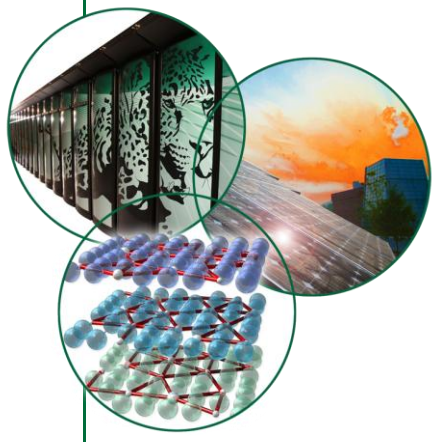
Modernization of SCALE

B. T. Rearden
Oak Ridge National Laboratory
Oak Ridge, TN



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OAK RIDGE NATIONAL LABORATORY
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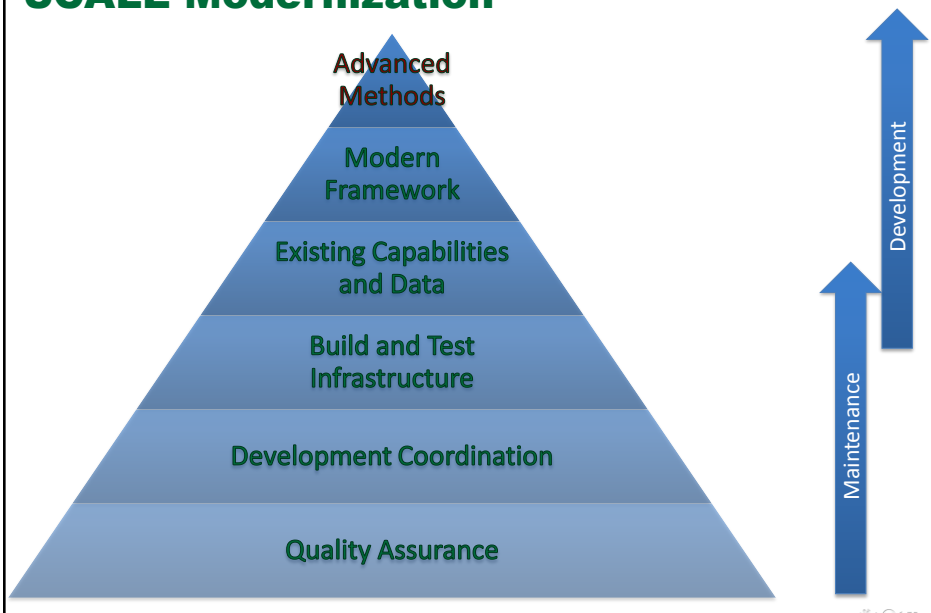
Legacy SCALE

- 89 executable modules that communicate through file I/O
  - More than a dozen data file formats
  - Internal scratch files
- Many features were initiated over 40 years ago (e.g. KENO) with other key capabilities introduced over past 20 years
  - Reliable, tried and true, but in need of review
- No parallel calculations, only serial (by design)
- Only capable of compiling with the Intel compilers (~$1000/license)
- 500K lines of Fortran code that is primarily tested with “sample” problems, not modern units tests
- Lots of duplicated code where a component is copied by a developer, slightly modified, and given a new purpose. Easy to get features out of phase with each other.
- Restrictive data file formats that are coded into each module, complicating introduction of new features
- “Code managers” given broad tasks that are loosely coordinated

Drive for Modernization

- Need to keep pace with evolving computer platforms and provide increased solution fidelity in reasonable wall-clock time through parallel computing
- Coordination of SCALE maintenance support (NCSP and others) and targeted development from many sponsors (NRC, DOE, DHS, etc) to provide best product for all users
- Legacy framework makes it increasingly difficult to integrate new features without breaking existing features
- Minimize duplication of effort
- Tight integration with other projects such as CASL
  - Provide great opportunities for feature enhancements, but place external expectations on software lifecycle
- Provide development environment suitable for a large team of next-generation developers

SCALE Modernization



SCALE Modernization

Quality Assurance Program

- Quality is a top priority, and an extensive quality program is used to govern the development and deployment process.
- Quality Plan
  - New SCALE QA plan was developed for compliance with:
  - ISO 9001
  - DOE 414.1C
  - NQA-1
  - ORNL Standards-Based Management System (SBMS)
- Enables “Agile” software development process following Kanban product lifecycle
- Plan to integrate AMPX under SCALE QA

SCALE Modernization

SCALE Leadership Team

- Coordinates overall vision for SCALE
- Sets priorities and reviews progress
- Meets weekly to maintain close coordination

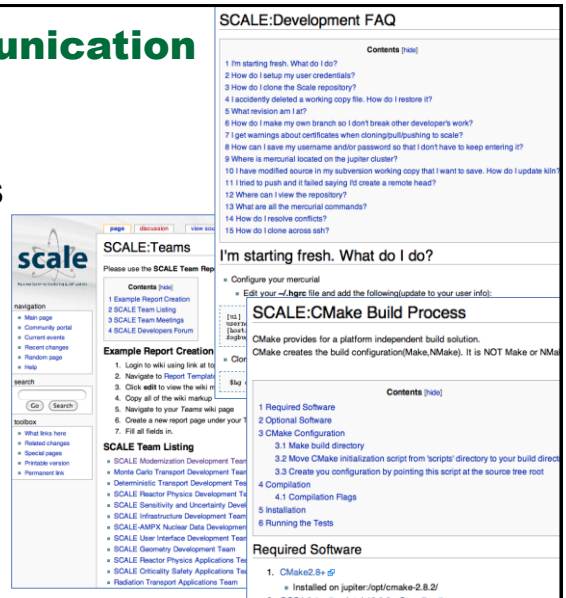
- John Wagner
  Design, Safety and Simulation Integration Manager
- Brad Rearden
  SCALE Project Leader
- Mike Dunn
  Nuclear Data and Criticality Safety Group Leader
- Bob Grove
  Radiation Transport Group Leader
- Steve Bowman
  Reactor Physics Group Leader
- Mark Williams
  Scale Computational Methods Lead

SCALE Teams

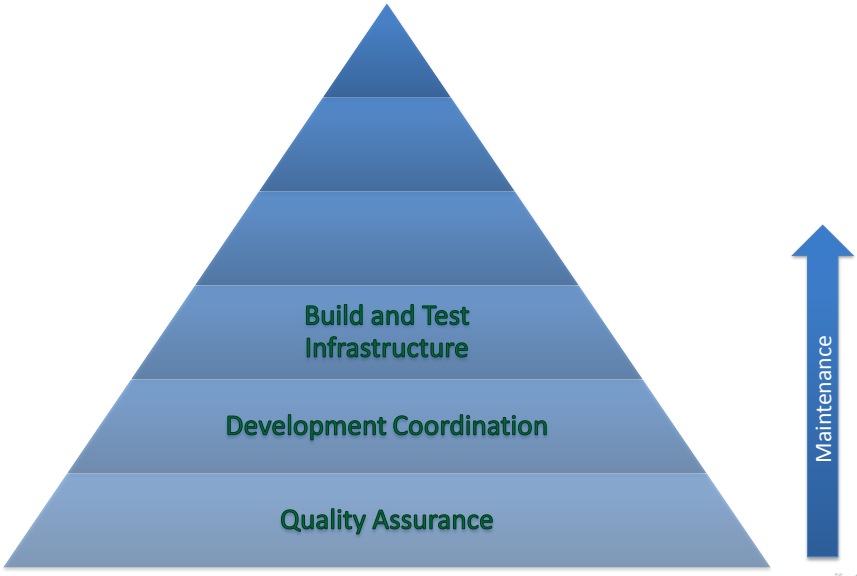
- SCALE Modernization Development Team
- SCALE Reactor Physics Development Team
- Monte Carlo Transport Development Team
- Deterministic Transport Development Team
- SCALE Sensitivity and Uncertainty Development Team
- SCALE Infrastructure Development Team
- SCALE-AMPX Nuclear Data Development Team
- SCALE User Interface Development Team
- SCALE Geometry Development Team
- SCALE Reactor Physics Applications Team
- SCALE Criticality Safety Applications Team
- Radiation Transport Applications Team

Developer Communication

- Team meetings
- Frequent project meetings
- Development sprints
- Wiki pages
- Friday Developers Forum
- War Room



SCALE Modernization



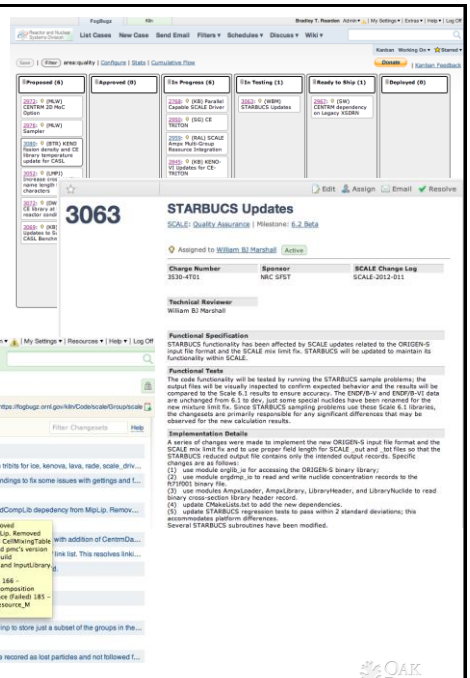
Build System

CMake
Cross-platform Make

- Same code and build system used on all platforms, Linux, Mac, Windows
- Supported platforms with pre-compiled binaries available on installation
  - Linux 32- and 64-bit
  - Mac 32- and 64-bit
  - Windows 32- and 64-bit

FogBugz

- Track QA feature development
- Helpline tickets and email
- Monitor changes to code repository



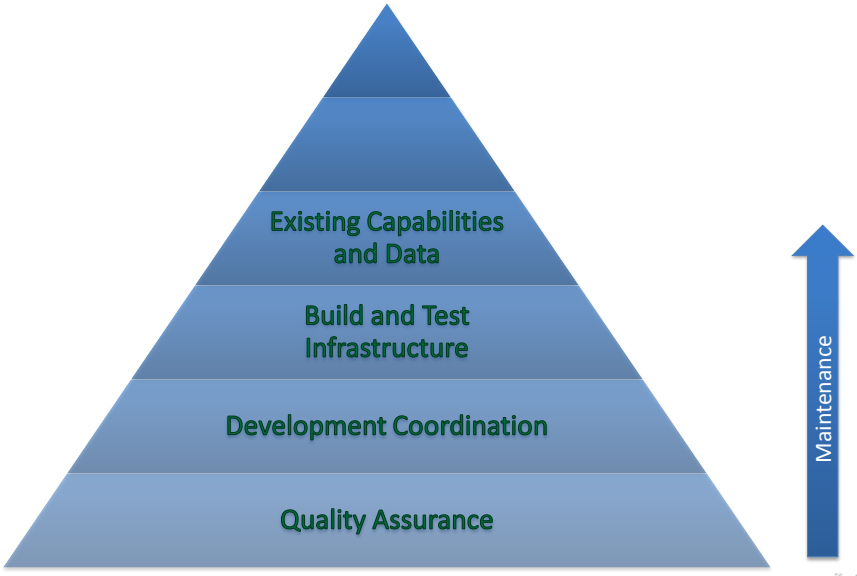
Test Harness and Dashboard

- After every update, SCALE is automatically built and tested to ensure functionality of all tested features
  - ~500 test cases (still need more)
  - Linux, Mac, Windows
  - Intel and GNU compilers
  - Release and Debug mode

Linux Regression

Site	Build Name	Update		Configure			Build			Test				Build Time	Labels
		Files	Min	Error	Warn	Min	Error	Warn	Min	NotRun	Fail	Pass	Min		
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	13	0.2	0	0	1.3	0	0 +10	5.6	0	4	477	221.6	2012-03-07T11:50:42 EST	(none)
node16.ornl.gov	LEGACY-RELEASE-Intel-12.0.3.174	11	0.4	0	0	3.4	0	16 +10	14.1	0	4	477	223.8	2012-03-07T07:48:54 EST	(none)

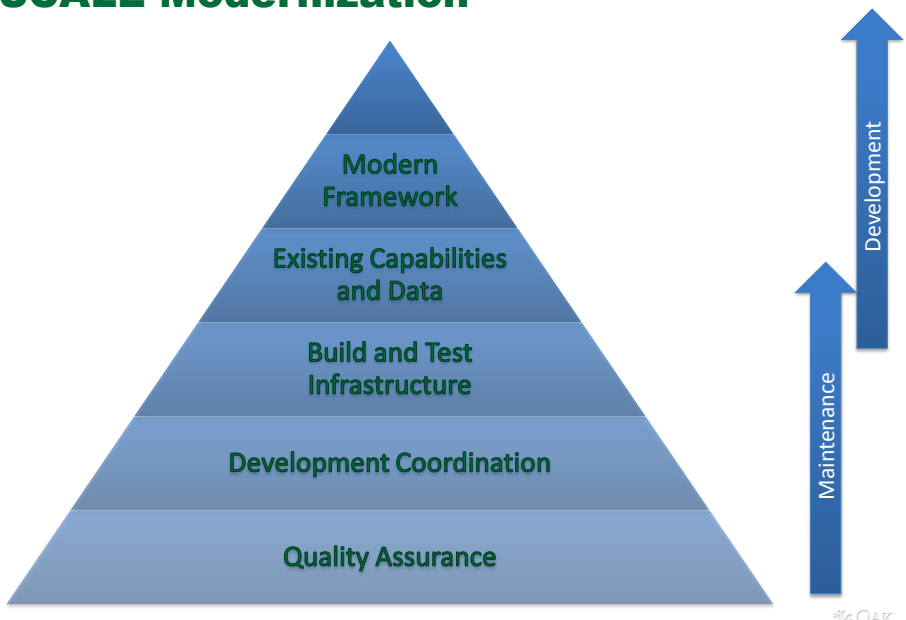
SCALE Modernization



Preservation of Current Capabilities

- Perform extended validation testing (see previous talk)
- Target areas for incremental improvement
- Develop verification regression tests to ensure needed features continue to perform as expected
- Remove seldom used features to reduce maintenance costs
  - ENDF/B-V, ENDF/B-VI data
  - QADS, PICTURE, MARSLIB, QADSCGGP
  - SMORES
  - NITAWL, NITAWLST
- Consolidate features to reduce maintenance cost
  - KENO V.a, KENO-VI, Monaco

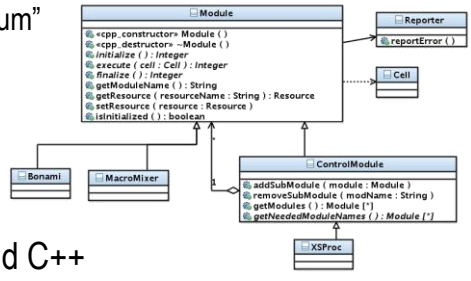
SCALE Modernization



SCALE 7 Framework

- Object-oriented C++ framework
- Allows multiple levels of parallel implementation
- Easy to implement modern development practices like unit tests, test-driven development, and Design by Contract
- Extensible base components
  - Centralized input processor "Fulcrum"
  - Modules for functionality
  - Resources for data
  - Reporter for output
  - Parallel driver and distributor
- Templates for binding Fortran and C++

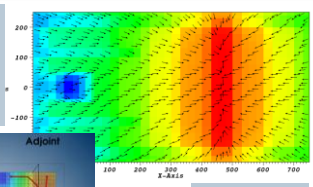
Module Logical Architecture Diagram



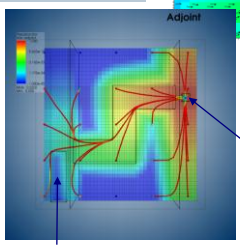
Denovo is a new, modern S_N RT code that takes advantage of decades of research/experience

- Originally developed to support hybrid methods, but has expanded well beyond that

Denovo provides adjoint data used to generate consistent mesh-based weight windows & source biasing parameters for accelerating MC calculations.



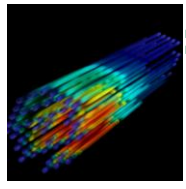
adjoint currents show preference from source to tally region



Tally region in forward problem

forward source region

- State of the art transport methods
  - 3D/2D, non-uniform, regular grid S_N
  - 2D MoC Solver
  - Multi-group energy, anisotropic P_N scattering
  - Forward/Adjoint
  - Fixed-source/*k*-eigenvalue
  - 6 spatial discretization algorithms
  - Parallel first-collision
  - Multiple quadratures
- Modern, Innovative, High-Performance Solvers

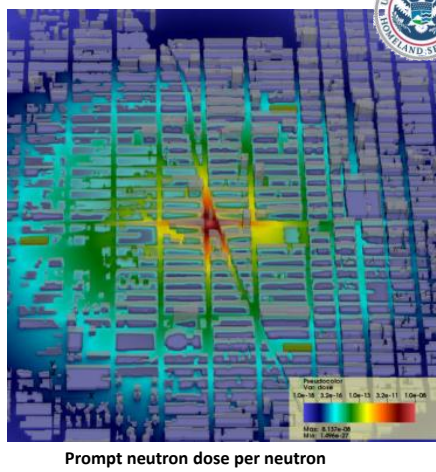


Power distribution in a BWR assembly0

Denovo is being used to solve enormous problems of national interest

Postulated nuclear detonation in Manhattan, NY

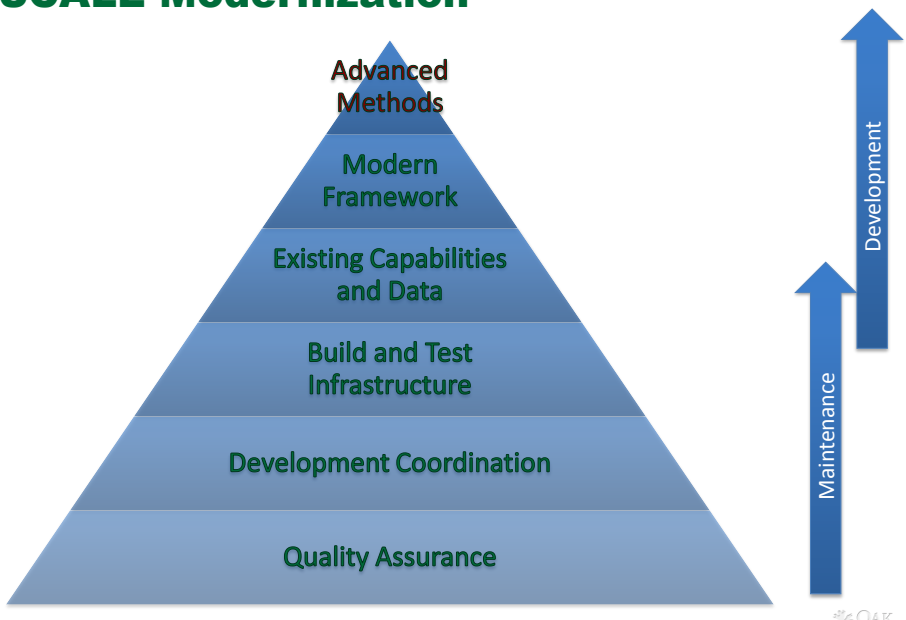
Num cells:	224,438,368
Num angles:	288
Num groups:	46
Num moments:	16
Num Unknowns in State:	1.36459e+11
Memory of State (GB):	1.27087e+02
Solved unknowns:	3.93001e+13
Cores:	10080
Wall-clock time (min):	1.79583e+01
CPU-HOURS:	3.01700e+03
Setup time (min):	1.15526e+00
Ray-tracing (min):	4.08660e-02
Solver time (min):	1.38992e+01
Output time (min):	2.90386e+00



Prompt neutron dose per neutron

> 224M spatial cells, 46 neutron groups, P_3 Scattering, S_{16} angular quadrature, full-field solution in < 18 minutes with 10,080 cores on JAGUAR (3,017 CPU-Hrs)

SCALE Modernization



XSProc

- First SCALE 7 tools for multigroup resonance self-shielding modules collectively known as XSProc
  - Fulcrum
  - "Cell" class
  - BONAMI
  - XSDRNPM
  - MixMacro
  - Dancoff
- OpenMP
- MPI

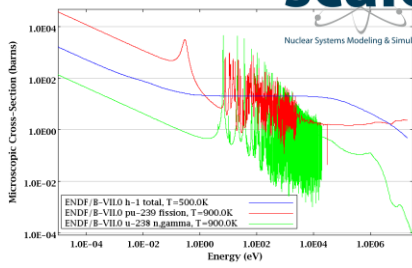
Time to Process Cross Sections for 102 Pin Cells on 8-Core Workstation

Processors	Execution Time (seconds)		
	SCALE 6.1 CENTRM	SCALE 6.1 BONAMI	XSProc
1	5167.20	749.48	193.00
2	N/A	N/A	121.98
3	N/A	N/A	94.10
4	N/A	N/A	84.74
5	N/A	N/A	75.90
6	N/A	N/A	70.34
8	N/A	N/A	63.89

- Integrated with CASL neutronics
- May provide self-shielding for SCALE 6.2

SCALE Cross Section Data Resource

- A unified nuclear cross section data Resource was developed for integration throughout SCALE and AMPX
- Objective: Remove restrictions on M&S capabilities that are imposed by archaic 40-year old binary data format that is used in more than 100 computational modules



Accomplishments

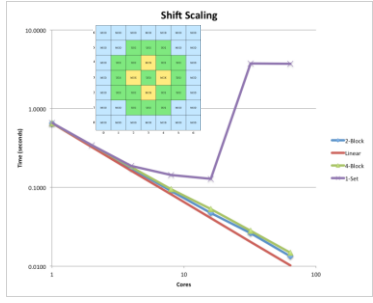
- Resource was implemented in key codes in SCALE to remove restrictions on number of materials and number of energy groups that were imposed by the previous file format that pre-dated the existence of SCALE.
  - Materials limit 2147 → new: 2,147,483,648
  - Energy groups limit 999 → new: 2,147,483,648
- Modern, dynamic, tested, object-oriented Resource was created to provide cross section data to any computational code in c, c++, or Fortran.
- Any new data features can be implemented in the centralized Resource for immediate availability to all Resource-enabled codes (e.g. subgroup parameters)

Impact

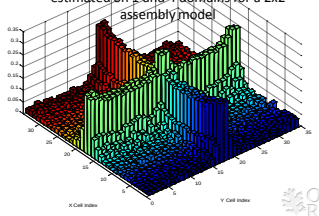
- ❑ Enables virtually unlimited materials and energy groups in SCALE calculations
- ❑ Enables dynamic updating of cross section data for future needs

New Domain-Decomposition Monte Carlo Code, *Shift*, Under Development

- Designed from outset for use on massively parallel platforms
  - Domain replication and domain decomposition
  - Parallel scaling studies on-going
- *SCALE* geometry (KENO-VI)
- Implementing hybrid methods
  (Shift + Denovo in common code base)
- Approaches for efficient variance estimation
  - Evaluating batches vs. neglecting variance contributions from particles that leave domains
- Implementing continuous energy physics
- Implemented Shannon Entropy
- Testing, verification and validation



Relative difference between variances estimated on 1 and 4 domains for a 2x2 assembly model



Shift Features and Wish List

Development Features

- P_0 multigroup physics using SCALE MG cross-sections
- Python scripts written by developers drive code input
- No output file, only binary data files
- Developed for reactor physics
- KENO-VI geometry
- Advanced multi-set overlapping-region domain-decomposition parallel capabilities
- FW-CADIS and advanced source convergence features (in progress)
- Advanced S/U methods (PhD dissertation)
- MCNP geometry (in progress)
- MCNP physics and data (in progress)

Needed Features

- User input
- User output
- SCALE CE physics
- SCALE MG physics
- KENO V.a geometry
- Criticality safety features like k_{eff} matrix edits
- Production S/U features in multigroup and continuous-energy
- Graphical user interface

Modernization To-Do List

- Targeted improvements realized though extended validation
- Continue to improve verification test coverage to include all SCALE features
- Integrate all cross section capabilities into XSProc
  - CENTRM Continuous-energy treatment
  - Double heterogeneity
  - 2D methods (not mentioned in this talk)
- Update Shift to include features of KENO, Monaco, and TSUNAMI-3D
- Integrate all code into SCALE 7 Framework for efficient parallel operation
- Release available features in SCALE 6.2

Shift Contributors and Acknowledgments

- Staff contributors:
  - Tom Evans
  - Josh Jarrell
  - Greg Davidson
  - Steven Hamilton
  - Kevin Clarno
  - John Wagner
  - Scott Mosher
  - Douglas Peplow
  - Bob Grove
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