OAK RIDGE National Laboratory

PO Box 2008
Oak Ridge, TN 37831-6172
(865) 323-8210 | SCALEHELP@ornl.gov

SCALE User Notice

Memory error with SCALE 3D general geometry package leading to an incorrect model when shapes are truncated by CHORDs

April 1, 2021

In SCALE 4.4-6.2.4 [1], the SCALE 3D General Geometry Package (SGGP) which provides the engine for "KENO-VI-style" geometry, may not correctly process the specification of multiple CHORD modifiers when defining a truncated shape. This problem occurs due to a memory error. **Tests with the official SCALE 6.2.4 release binaries for Linux and Mac result in an abrupt termination of the calculation. Release binaries for Windows appear to use the user-intended geometry, but caution is advised given the behavior is compiler-specific and the underlying error is still present in the code.** With a user-compiled executable of SCALE 6.2.4 that was created at Oak Ridge National Laboratory (ORNL) on Linux and Mac OS platforms using recent GNU compilers, the calculation proceeds, and unintended geometry changes cause unpredictable effects in the neutron multiplication factor, k_{eff}, neutron and/or photon fluxes, and any associated tallies/responses. We consider this a significant software error, since (1) large errors in computed results are possible, and (2) the SCALE test suite does not currently include any test case that uses the minimum number of CHORD modifiers necessary to activate the defect. For users of sequences downstream of SGGP, including CSAS6, MAVRIC, TRITON (t6-depl), TSUNAMI (tsunami-3d-k6), STARBUCS (with KENO-VI geometry), and MCDANCOFF, who have built SCALE from source, the recommendation is to run the sample problems provided herein and to examine the results. **Note this error does not affect CSAS5 which uses KENO V.a.**

The underlying cause of this error is a static array in the SGGP geometry processor which may be exceeded when CHORDs are used. User-defined shapes are translated into a set of quadratic equations, and their coefficients are stored in this array and sized for six-surface equations, which is sufficient for any shape. However, truncation with a CHORD modifier adds an additional surface equation, and depending on the shape, it may exceed the bounds of the array and cause undefined behavior. The same effect was found with almost all predefined shapes available in SGGP when truncating them with one or more CHORD modifiers, depending on the shape type. The bias observed in the calculated k_{eff} for the considered test cases was in the range 0–25%, but given the nature of the error, larger biases may be possible.

Per the requirements of the Quality Assurance Plan for the SCALE Code System [2] and specifically the SCALE Procedure for Discrepancy Reports [3], this defect is being categorized as a *Significant Software Error* and is reported in this User Notice.

Director, SCALE Code Suite

April 1, 2021
Date

1. Summary

A defect has been found in SCALE 4.4-6.2.4 in which the shape truncation by a single or multiple CHORD modifier(s) can cause significant bias due to the surface coefficient static array size being exceeded. For example, geometry defined with a sphere with multiple CHORD modifiers resulted in an unexpected eigenvalue compared to the results from the other two models, as presented in the table below. As expected, results from the Godiva sphere and a slightly truncated Godiva sphere ("forged Godiva") are not the same, but they show only a small difference. **However, the "forged Godiva" obtained with multiple CHORD modifiers produces a result with a large bias**.

The following inputs illustrate the geometry configurations used in this summary of the error. Any SCALE sequence which uses the SGGP geometry processor is affected, including CSAS6, MAVRIC, TRITON, TSUNAMI, STARBUCS and MCDANCOFF with "KENO-VI-style" geometry. **The plot block included in the inputs below will show the internal geometry and can be used to visually verify if the defect is present.**

```
=csas6
Godiva sphere
ce_v7.1
read composition
 u-234       1 0 0.000491995 293   end
 u-235       1 0 0.0449996 293   end
 u-238       1 0 0.002498 293   end
end composition
read parameter
  htm=no npg=10000
end parameter
read geometry
global unit 1
    sphere  30 8.741
    media 1 1 30
  boundary 30
end geometry
read plot
  ttl="Original godiva, X-Z cut"
  lpi=10 scr=yes
  xul=-9 yul=0 zul=9.0
  xlr=9 ylr=0 zlr=-9.0
  uax=1 wdn=-1.0
  nax=1000 pic=mat end plt1

  ttl="Original godiva, X-Y cut"
  lpi=10 scr=yes
  xul=-9 yul=9 zul=.0
  xlr=9 ylr=-9 zlr=.0
  uax=1 vdn=-1.0
  nax=2000 pic=mat end plt2
end plot
end data
end
```

Figure 1. Godiva sphere.

```
=csas6
Godiva sphere forged on 6 sides, sphere truncated by a cuboid
ce_v7.1
read composition
 u-234       1 0 0.000491995 293   end
 u-235       1 0 0.0449996 293   end
 u-238       1 0 0.002498 293   end
end composition
read parameter
  htm=no npg=10000
end parameter
read geometry
global unit 1
    sphere  30 8.741
    cuboid  20 6p8.3
    media 1 1 30 20
    media 0 1 20 -30
boundary 20
end geometry
read volume type=random end volume
read plot
  ttl="Forged godiva truncated by a cuboid, X-Z cut"
  lpi=10 scr=yes
  xul=-9 yul=0 zul=9.0
  xlr=9 ylr=0 zlr=-9.0
  uax=1 wdn=-1.0
  nax=1000 pic=mat end plt1

  ttl=" Forged godiva truncated by a cuboid, X-Y cut"
  lpi=10 scr=yes
  xul=-9 yul=9 zul=.0
  xlr=9 ylr=-9 zlr=.0
  uax=1 vdn=-1.0
  nax=2000 pic=mat end plt2
end plot
end data
end
```

Figure 2. “Forged Godiva,” truncated by a cuboid.

```
=csas6
Godiva sphere forged on 6 sides, sphere truncated by six CHORD modifiers
ce_v7.1
read composition
 u-234       1 0 0.000491995 293   end
 u-235       1 0 0.0449996 293   end
 u-238       1 0 0.002498 293   end
end composition
read parameter
  htm=no npg=10000
end parameter
read geometry
global unit 1
    sphere  30 8.741 chord +x=-8.3 chord -x=8.3
                     chord +y=-8.3 chord -y=8.3
                     chord +z=-8.3 chord -z=8.3
    media 1 1 30
  boundary 30
end geometry
read volume
   type=random
end volume
read plot
  ttl="Forged godiva truncated by six CHORDs, X-Z cut"
  lpi=10 scr=yes
  xul=-9 yul=0 zul=9.0
  xlr=9 ylr=0 zlr=-9.0
  uax=1 wdn=-1.0
  nax=1000 pic=mat end plt1

  ttl="Forged godiva truncated by six CHORDs, X-Y cut"
  lpi=10 scr=yes
  xul=-9 yul=9 zul=.0
  xlr=9 ylr=-9 zlr=.0
  uax=1 vdn=-1.0
  nax=2000 pic=mat end plt2
end plot
end data
end
```

Figure 3. "Forged Godiva," truncated by six CHORDs.

Table.1 k_{eff} results of different Godiva sphere specification (results were obtained with a custom SCALE 6.2.4 build produced with GNU-8.4 compilers on a Mac system)

Model	k_{eff}
Godiva sphere (original, no truncation)	1.000410 +/- 0.000630
Godiva sphere pressed on 6 sides (truncated with a cuboid)	0.997550 +/- 0.000740
Godiva sphere pressed on 6 sides (truncated with 6 CHORDs)	**0.758930** +/- 0.000650

These results confirm that the SGGP geometry processor has a defect with a predefined shape with multiple CHORD modifiers. When examining the geometry edits in the code output, it can easily be seen that the SGGP geometry processor incorrectly sets up the last quadratic equation (which is the translation of surface specified by the last CHORD operation, chord -z=8.3).

```
      1         sphere         30                           quadratic surfaces

      X**2          Y**2          Z**2          XY          XZ          YZ          X
Y            Z      Constant

  -1.00000E+00 -1.00000E+00 -1.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00
+0.00000E+00 +0.00000E+00 +7.64051E+01

  +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +1.00000E+00
+0.00000E+00 +0.00000E+00 +8.30000E+00

  +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00
-1.00000E+00 +0.00000E+00 +0.00000E+00 +8.30000E+00

  +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00
+1.00000E+00 +0.00000E+00 +8.30000E+00

  +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 -
1.00000E+00 +0.00000E+00 +8.30000E+00

  +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00
+0.00000E+00 +1.00000E+00 +8.30000E+00

  +3.39519-313 +2.19295-314 +7.95446-322 +0.00000E+00 +0.00000E+00 +0.00000E+00 +0.00000E+00
+0.00000E+00 -1.00000E+00 +0.00000E+00
```

Figure 4. Excerpt from the output file showing "Forged Godiva" quadratic surface coefficients illustrating incorrect chord coefficients in bold red.

The SGGP geometry engine with this incorrect quadratic equation performs a truncation at z=0.0 instead of at z=8.3. In other words, half of the Godiva sphere is truncated; the code performs the transport calculation inside this hemisphere rather than inside the full sphere, resulting in almost 25 %Δk bias in the results.

The error is not visible in Fulcrum visualization as it uses a different geometry engine than SGGP. Fulcrum displays all of these geometries as expected, as shown in Figure 5.

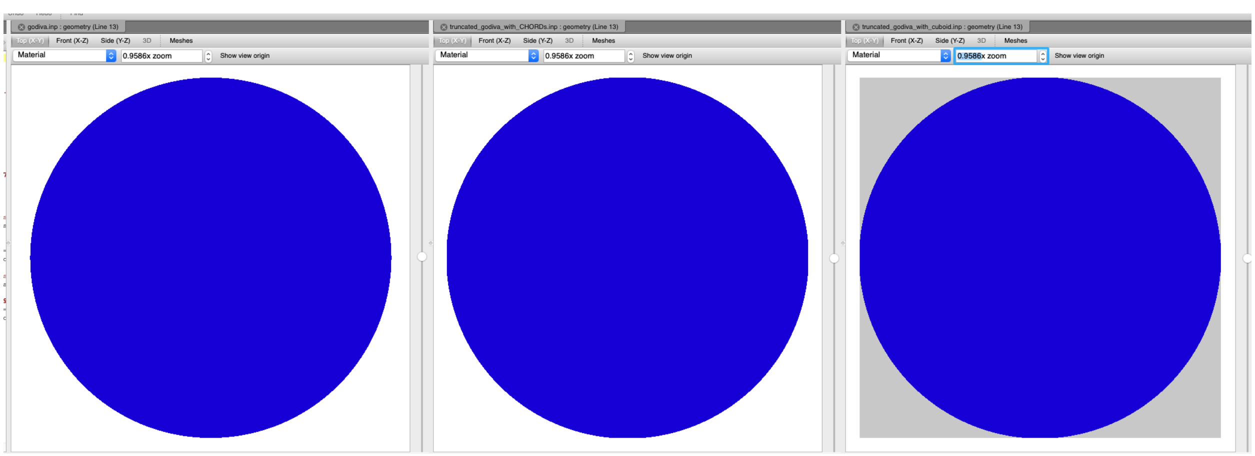

Figure 5. Fulcrum geometry visualization: Godiva sphere, untruncated (left), "Forged Godiva" truncated by six chords, no error shown (center), and "Forged Godiva" truncated by cuboid (right).

Unlike Fulcrum, the discrepancies in the processed geometry specification can easily be seen with the integrated SCALE plotter (activated by the PLOT block), as shown in Figure 6.

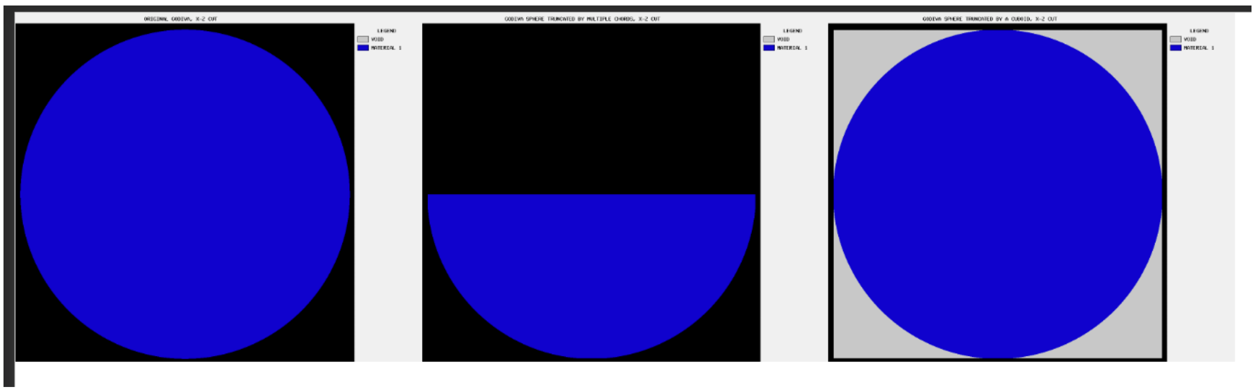

Figure 6. KENO-VI plotted geometry: Godiva sphere, untruncated (left), "Forged Godiva" truncated by six chords, error shown (center), and "Forged Godiva" truncated by cuboid (right).

2. Recommended Actions

Users should review their SGGP geometry chord use to ensure that the maximum occurrence of CHORD modifier is not exceeded for any shape. Table 2 provides the number of quadratic equations used for each unmodified shape, and the number of CHORD modifiers that must be used to trigger the defect. Use of fewer than the specified number of CHORD modifiers guarantees that the error will not be encountered. **A review of the image generated from a PLOT block can also indicate whether a problem exists.** This SCALE plot image accurately reflects the geometry for subsequent transport calculations. In some cases, the effect of the CHORD modifiers may be recreated with an intersecting shape, such as a CUBOID, and the appropriate modification of the relevant MEDIA records. For "Forged Godiva," an example using the CUBOID to achieve a similar effect is shown in Figure 2. In other cases, instead of using CHORD modifiers, PLANES can be used with the appropriately updated MEDIA records to perform the equivalent truncation.

Table 2. SGGP shape quadratic surface count and required chord count to exceed memory limit

Shape	Number of quadratic equations for unmodified shape	Number of CHORD modifiers to trigger defect
sphere	1	6
ellipsoid	1	6
plane	1	6
xpplane	1	6
ypplane	1	6
zpplane	1	6
quadratic	1	6
cone	2	5
cylinder	2	5
ecylinder	2	5
xcylinder	2	5
ycylinder	2	5
zcylinder	2	5
ring	3	4
cuboid	3	4
parallelepiped	3	4
rhomboid	3	4
hexprism	4	3
rhexprism	4	3
wedge	4	3
hopper	5	2
pentagon	6	1
dodecahedron	6	1

3. Details

This defect was originally reported by an internal user in a model in which the geometry specification of a HOPPER resulted in unexpected results when both ends of this object were truncated with CHORD modifiers. This result was only observed when running this input with a custom SCALE 6.2.4 build on a Mac system. Later, the same error mode was reproduced with a custom SCALE 6.2.4 build on a Linux system.

Our investigations indicate that SGGP has a memory defect which resulted in an incorrect interpretation of the truncations made by multiple CHORD modifiers for almost all predefined shapes allowable in SGGP geometry. SGGP defines each geometric shape with a set of quadratic equations with 11 coefficients. User-specified shapes are translated into a set of quadratic equations, and the coefficients of these equations are stored in a static array. Truncation made by a CHORD modifier defines a new surface for the shape, so it is translated into another quadratic equation, and its coefficients are also stored in the same static array. Unfortunately, the size of this array was limited so that it only stores the coefficients for up to six quadratic equations. This array storage size can be easily exceeded when defining multiple `CHORD` modifiers to a predefined shape, and this results in an unexpected surface definition for the truncated shape.

Table 2 summarizes the predefined shapes and the number of quadratic equations required to specify them. The corresponding number of CHORD modifiers required to exceed the surface array memory limit is also provided.

According to Table 2, all these shapes with multiple CHORD modifiers may cause incorrect interpretation in geometry setup **if and only if the total number of quadratic equations (sum of the number of equations used to specify the predefined shapes and the number of CHORD modifiers) is greater than 6**. Therefore, in the original problem, a HOPPER truncated at both the top and bottom ends produced incorrect results since the last (7^{th}) quadratic equation cannot be stored properly in the allocated space. Similarly, the "forged Godiva" case introduced and discussed above has a total of 7 quadratic equations, and the allocated space is insufficient to store the coefficients of the last (7^{th}) quadratic equation. Since complex shapes are affected by fewer CHORD modifiers, users are encouraged to examine complex shapes first.

- The PENTAGON and the DODECAHEDRON may be affected by 1 CHORD.
- The HOPPER may be affected by 2 CHORDs.
- The WEDGE, HEXPRISM, and RHEXPRISM may be affected by 3 CHORDs.
- The RHOMBOID, PARALLELEPIPED, CUBOID, and RING (and variants) may be affected by 4 CHORDs.
- The CYLINDER (and variants), and CONE may be affected by 5 CHORDs.
- The SPHERE, ELLIPSOID, PLANE, PPLANE variants, and QUADRATIC may be affected by 6 CHORDs.

All of our investigations showed that this defect caused a significant bias (up to 25 %Δk for the "forged Godiva" model) on both Mac and Linux systems if SCALE 6.2.4 had been built with one of the recent GNU Fortran compilers. **None of the SCALE 6.2.4 release binaries prepared for Linux, Mac, or Windows platforms** was able to reproduce this defect.

Table 3. Checklist for significant software error notification

Item	Description
Software identification	• Sequences: CSAS6, MAVRIC, TRITON (t6-depl), TSUNAMI (tsunami-3d-k6), STARBUCS (with KENO-VI geometry), and MCDANCOFF which rely on the SGGP geometry module • Version impacted: SCALE 6.2 (CCC-834) and subsequent updates 6.2.1, 6.2.2, 6.2.3, 6.2.4 • Previous SCALE versions which **WERE NOT TESTED** but are known to include the faulty source code include SCALE 6.1, 6.1.1, 6.1.2, and 6.1.3; SCALE 6; SCALE 5.1; SCALE 5; and SCALE 4.4. Testing was not undertaken given the uncertainty in compatibility of the current generation of compilers with the older code base. • The NEWT 2D geometry engine is separate from SGGP and uses allocatable arrays and is not affected.
Data library	The defect is present without regard to the data library selected.
Computing platform (Unix, Windows, Linux, etc.)	The defect is present in source and thus potentially affects all platforms, but it has only been observed to produce unexpected geometry truncations on both Linux and Mac operating systems with rebuilds of SCALE 6.2 from source with recent GNU compilers with "release" flags and optimizations (i.e., not "debug").
Description of the error	An error occurs in the SGGP geometry processor, causing the addition of CHORD modifiers to truncate geometry in unexpected ways.
How was the error identified?	An ORNL internal user reported unexpected behavior related to the use of 2 CHORD modifiers on a HOPPER shape. Further investigation uncovered the underlying defect.
When does this error occur?	Any SGGP shape for which the number of quadratic equations exceed 6 will exploit the memory defect and may result in unacceptable bias: • The PENTAGON and the DODECAHEDRON may be affected by 1 CHORD. • The HOPPER may be affected by 2 CHORDs. • The WEDGE, HEXPRISM, and RHEXPRISM may be affected by 3 CHORDs. • The RHOMBOID, PARALLELEPIPED, CUBOID, and RING (and variants) may be affected by 4 CHORDs. • The CYLINDER (and variants), and CONE may be affected by 5 CHORDs. • The SPHERE, ELLIPSOID, PLANE, PPLANE variants, and QUADRATIC may be affected by 6 CHORDs.

Table 3. Checklist for significant software error notification

Item	Description
Potential impact of this error	The magnitude of the error is problem dependent. The impact of the memory defect manifests as the unexpected removal of geometry. Therefore, the impact is related to how much material was neglected in the problem and the nature of the removed material.
Frequency/likelihood of this error occurring	The most likely scenario for experiencing this error is when using PENTAGON, DODECAHEDRON, or HOPPER shapes. These shapes are less commonly used and are infrequently combined with CHORDs.
How can users determine if this error affects their calculations?	Review your problem output's quadratic shape edit and determine whether any coefficient appears to be incorrect (e.g., 2e-322). Plotting suspect geometry with the native PLOT block within SCALE will also display the geometry as used for the transport calculation.
What action should users take if this error affects them?	The CHORD specification that is manifesting an error can be replaced with a plane, and the relevant MEDIA records can be updated appropriately.
Is correction to code/data available?	SCALE 6.3.0 will include error checking to prevent this memory defect from being exploited.
How to obtain/install correction	Users can check for and correct any noncompliant input immediately. SCALE 6.3.0 will be announced to the user distribution list in 2021 when it is released.

4. SCALE Quality Assurance Program

After the 2011 release of SCALE 6.1 [4], the SCALE Quality Assurance Program, associated procedures, and supporting infrastructure were substantially upgraded in 2013 as an essential starting point to SCALE modernization activities. As part of the ongoing modernization initiative, the SCALE team is continually seeking means of self-improvement.

5. References

1. W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., SCALE Code System, ORNL/TM-2005/39, Version 6.2.4, UT-Battelle, LLC, Oak Ridge National Laboratory (2020).

2. B. T. Rearden, M. T. Sieger, S. M. Bowman, and J. P. Lefebvre, Quality Assurance Plan for the SCALE Code System, SCALE-QAP-005, Rev. 4, Oak Ridge National Laboratory (2013).

3. B. T. Rearden, J. P. Lefebvre, and S. M. Bowman, SCALE Procedure for Discrepancy Reports, SCALE-CMP-004, Rev. 5, Oak Ridge National Laboratory (2013).

4. SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, UT-Battelle, LLC, Oak Ridge National Laboratory (2011).