

Sampler examples for nuclear criticality safety applications

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Learning goals

- Understand the input and structure of placeholders in Sampler
- Understand the input and structure of parametric capabilities in Sampler
- Understand the input structure of Sampler for use with the workshop: Data sampling and comparison to TSUNAMI-1D results

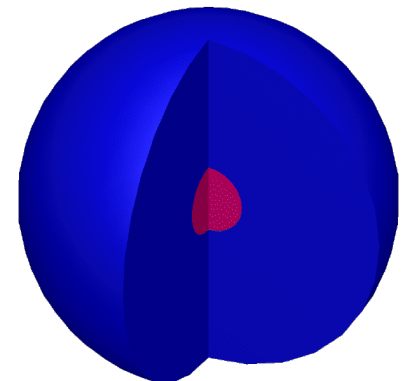
Data sampling and comparison to TSUNAMI-1D results

- Workshop 1



Objectives

- Develop Sampler input for nuclear data perturbations from the KENO input provided
- Run a (small) series of different perturbations to get a rough estimate of the uncertainty in k_{eff} resulting from nuclear data uncertainty
- Compare Sampler uncertainty estimate of k_{eff} with TSUNAMI-1D estimate of nuclear data-induced uncertainty in k_{eff}



Steps

1. Find CSAS5 input for HMF-004
2. Create Sampler sequence input
 - Embed the HMF-004 input in a case block
 - Add response block
3. Run Sampler
 - Sampler will run CSAS cases
4. TSUNAMI-1D data-induced uncertainty estimate is 1.09% Δk

Data sampling and comparison to TSUNAMI-1D results

- Workshop 1 solutions



CSAS5 input

```
=csas5
HEU Sphere inside Sphere of Water
v7.1-252
read comp
u-234 1 0 5.3678-4 end
u-235 1 0 4.7033-2 end
u-236 1 0 9.5896-5 end
u-238 1 0 4.7782-4 end
h 2 0 6.6807-2 end
o 2 0 3.3403-2 end
end comp
read cell
multiregion spherical end
1 6.5537
2 33.471
end zone
end cell
read param
    htm=no
end param
read geometry
global unit 1
    sphere 1 1 6.5537
    sphere 2 1 33.471
end geometry
end data
end
```

Sampler parameter block

```
=sampler  
,  
read parameters  
  n_samples=10  
  perturb_xs=yes  
  library="v7.1-252n"  
end parameters
```

Sampler creates 10 complete CSAS inputs with different perturbed data and runs them.

OR

```
=sampler  
,  
read parameters  
  n_samples=10  
  perturb_xs=yes  
  run_cases=no  
  library="v7.1-252n"  
end parameters
```

Sampler creates 10 complete CSAS inputs with different perturbed data but doesn't run them. This may be more convenient on clusters with queuing systems.

Case block

```
read case[hmf_004]
sequence=csas5
HEU Sphere inside Sphere of Water
v7.1-252
read comp
u-234 1 0 5.3678-4 end
u-235 1 0 4.7033-2 end
u-236 1 0 9.5896-5 end
u-238 1 0 4.7782-4 end
h 2 0 6.6807-2 end
o 2 0 3.3403-2 end
end comp
read cell
multiregion spherical end
1 6.5537
2 33.471
end zone
end cell
read param
  htm=no
end param
read geometry
global unit 1
  sphere 1 1 6.5537
  sphere 2 1 33.471
end geometry
end data
end sequence
end case
```

Response block

```
read response[keff]
  type = grep
  regexp = ":kenova.keff:"
  eregexp = ":kenova.keff:"
end response

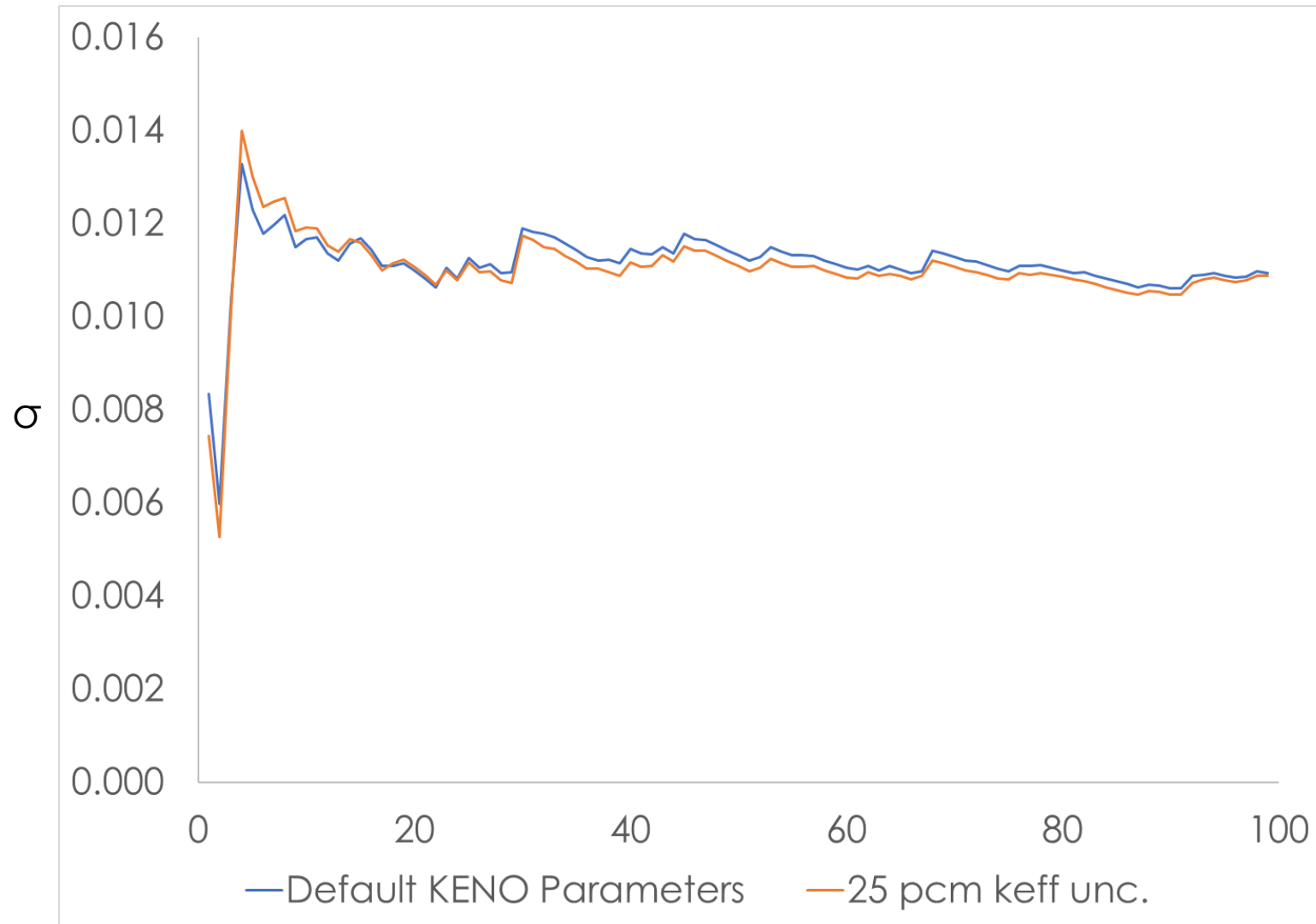
end
```

Standard deviation of k_{eff}

# of cases, KENO parameters	k_{eff} standard deviation (% Δk)
10, default	1.15
100, default	1.10
100, 25 pcm k_{eff} uncertainty	1.09

TSUNAMI-1D Result: 1.09%

Convergence of standard deviation estimate



Perturbation of compositions and geometry with placeholders



Objectives

- Understand variable placeholders in input
- Understand the 3 distributions available for sampling in variable blocks
- Understand how to generate expression variable blocks

Input placeholders

- Syntax: variable name inside braces with a pound sign prefix
`#{variable}`
- Variable must be defined in variable block (following slides)
- Variable names can have:
 - Letters (case sensitive)
 - Numbers
 - Underscores
 - No hyphens
 - Must start with a letter

Placeholders (aka Embedded Input)

SCALE Standard Composition

```
read composition
uranium      1 den=18.742 1 300
          92235 93.7112
          92238 5.2686
          92234 1.0202    end
end composition
```

Placeholder Variables

```
read composition
uranium      1 den=18.742 1 300
          92235  #{u235_wo}
          92238  #{u238_wo}
          92234  #{u234_wo}    end
end composition
```

Variable blocks

- Each variable is defined in its own block
 - No limit to number of variable blocks
- Each variable block contains:
 - Variable name
 - Distribution type (more later)
 - Distribution parameters
 - Cases in which variable is used
 - May contain SIREN statement
 - SIREN allows sampling without placeholders so that input is not changed
 - Not covered here due to time limitations

Variable block examples

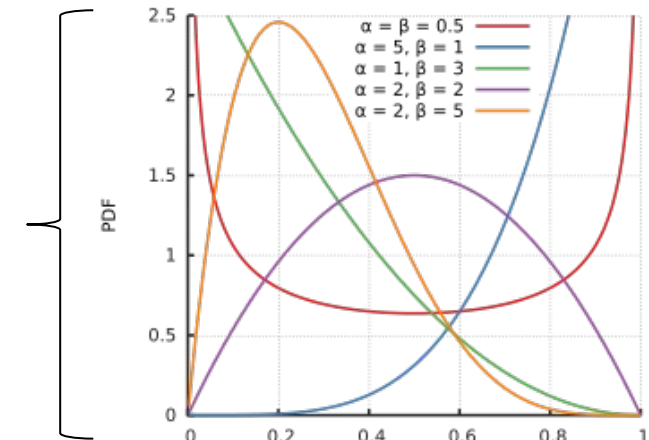
```
read variable[u235_wo]  
  distribution=normal  
  value=93.7112  
  stddev=0.05  
  min=93.5  
  max=93.9224  
  cases= godiva end  
end variable
```

```
read variable[u234_wo]  
  distribution=uniform  
  value=1.0202  
  min=1  
  max=1.0404  
  cases= godiva end  
end variable
```

```
read variable[u238_wo]  
  distribution=expression  
  expression = "100 - u235_wo - u234_wo"  
  cases= godiva end  
end variable
```

Distributions in Sampler

- 4 options for *distribution*= in a variable block
 1. Normal
 - Gaussian with specified average and standard deviation
 - Can be truncated
 2. Uniform
 - Constant probability between max and min
 3. Beta
 - Tunable distribution with 2 free parameters (α & β)
 4. Can also define an expression



Normal distribution

- Data input for normal distribution
- Keyword (*distribution=normal*)
- Mean value (*value=*)
 - Also used as nominal value
- Standard deviation (*stddev=*)
- Optional maximum and/or minimum values
 - *maximum=* and/or *minimum=*
- Cases to which the variable applies (*cases=*)

```
read variable[u235_wo]  
  distribution=normal  
  value=93.7112  
  stddev=0.05  
  min=93.5  
  max=93.9224  
  cases= godiva end  
end variable
```

Uniform distribution

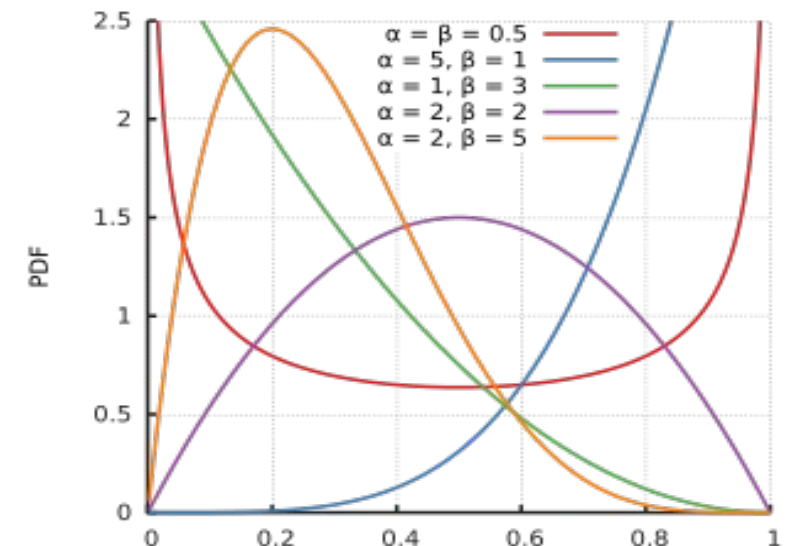
- Data input for uniform distribution
- Keyword (*distribution=uniform*)
- Nominal value (*value=*)
- Upper and lower bounds of distribution
 - *maximum=* and *minimum=*
- Cases to which the variable applies (*cases=*)

```
read variable[u234_wo]  
  distribution=uniform  
  value=1.0202  
  min=1  
  max=1.0404  
  cases= godiva end  
end variable
```

Beta distribution

- Data input for beta distribution
- Keyword (*distribution=beta*)
- Mean value (*value=*)
 - Also used as nominal value
- First (α) and second (β) parameters for distribution
 - *beta_a=* and *beta_b=*
- Upper and lower bounds of distribution
 - *maximum=* and *minimum=*
- Cases to which the variable applies (*cases=*)

```
read variable[plex_t5]  
  distribution = beta  
  beta_a = 4  
  beta_b = 2  
  minimum = 0  
  value = 0.296  
  maximum = 0.394667  
  cases = Case5 end  
end variable
```



Expressions

```
read variable[u238_wo]  
  distribution=expression  
  expression = "100 - u235_wo - u234_wo"  
  cases= godiva end  
end variable
```

- Variable block is largely the same
- Keyword (*distribution=expression*)
- Expression definition (*expression*="...")
- Definition includes variable names and math operators
 - Remember that variable names are case-sensitive
 - Math operators listed in section [6.4.7 of the SCALE Manual](#)
- Cases to which the variable applies (*cases*=)

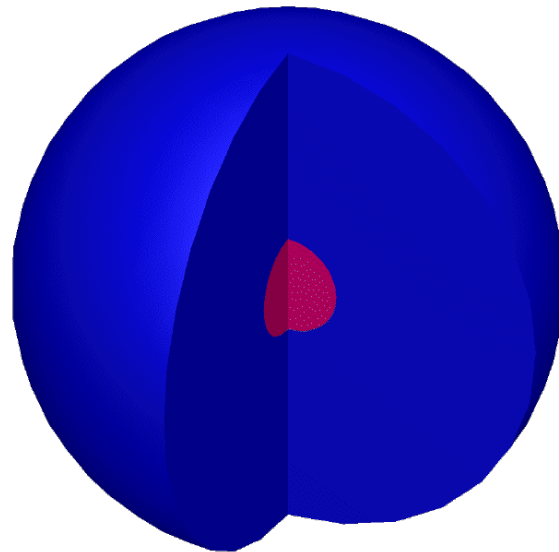
Compositions and geometry with placeholders

- Workshop 2



Objectives

- Develop Sampler input for composition perturbations from the KENO input provided
- Run a (small) series of different perturbations to get a rough estimate of the uncertainty in k_{eff} resulting from density and water density uncertainties



Steps

1. Open *hmf004-comp_sampling_STARTER.inp* from the workshop 2 folder
2. Add placeholders
3. Create variable blocks corresponding to the variable definition on the following slides
4. Run Sampler

Variables and assumed distributions

- Density of uranium metal
 - $18.794 \pm 0.010 \text{ g/cm}^3$
 - Assume uniform distribution, provided uncertainty represents 1σ
 - No basis, just to practice with more types
- Density of water
 - Assume beta: $\alpha=2$, $\beta=2$; nominal=0.99927; max=0.99954; min=0.99900
 - No basis, just to practice with more types

Implementation of perturbations

- Sample on U density
- Sample on H₂O density
 - Perturbation of water density requested while composition block contains explicit nuclide densities of H and O
- Calculate new H and O number densities
 - Realize nuclide density perturbations through the use of expression variable blocks
- Equations and basic data provided on next slide

Water

Isotope	Molar mass
^1H	1.007825
^{16}O	15.99491
Avogadro's Number	6.022142×10^{23}

$$M_{H_2O} = 2M_{^1H} + M_{^{16}O}$$

$$N_H = \frac{\rho_{H_2O} \times N_{Avo} \times 2 \frac{\text{atoms}}{\text{molecule}}}{M_{H_2O}}$$

$$N_O = \frac{\rho_{H_2O} \times N_{Avo}}{M_{H_2O}}$$

Compositions and geometry with placeholders

- Workshop 2 solutions



Addition of placeholders in comp block

```
read comp
u 1 den=18.794 1 293
    92234 1.17
    92235 97.67
    92236 0.20
    92238 0.96 end
H-1 2 0 6.6807-2 end
O-16 2 0 3.3403-2 end
end comp
```



```
read comp
u 1 den=#{u_dens} 1 293
    92234 1.17
    92235 97.67
    92236 0.20
    92238 0.96 end
h 2 0 #{ND_h} end
o 2 0 #{ND_o} end
end comp
```

Variable blocks to sample U density

```
read variable[u_dens]  
  distribution=uniform  
  value=18.794  
  minimum=18.784  
  maximum=18.804  
  cases = hmf_004 end  
end variable
```

Variable block to sample water density

```
read variable[O16_atomic_mass]
  distribution=expression
  expression="15.9949"
  cases = hmf_004 end
end variable
read variable[H1_atomic_mass]
  distribution=expression
  expression="1.007825"
  cases = hmf_004 end
end variable
read variable[avogadro]
  distribution = expression
  expression = "0.6022142"
  cases = hmf_004 end
end variable
```

```
read variable[water_dens]
  distribution=beta
  beta_a=2 beta_b=2
  minimum=0.99900
  value=0.99927
  maximum=0.99954
  cases= hmf_004 end
end variable

read variable[M_water]
  distribution=expression
  expression="2*H1_atomic_mass +
O16_atomic_mass"
  cases= hmf_004 end
end variable
```

Variable blocks to calculate ND_h and ND_o (Expression)

```
read variable[ND_h]  
  distribution=expression  
  expression="water_dens * avogadro * 2 / M_water"  
  cases= hmf_004 end  
end variable
```

```
read variable[ND_o]  
  distribution=expression  
  expression="water_dens * avogadro / M_water"  
  cases= hmf_004 end  
end variable
```

Standard deviation of k_{eff}

# of cases, KENO parameters	Average k_{eff}	k_{eff} standard deviation (Δk)
10, default	1.0007	0.00154
100, 25 pcm k_{eff} uncertainty	0.99904	0.00028

This small difference is on the order of the Monte Carlo uncertainties. Larger uncertainties would obviously increase the integral uncertainty.

Parametric studies



Objective

- Understand parametric capabilities of Sampler

Capability

- Parametric capability added in SCALE 6.2.2
- Sampling framework is repurposed to provide parametric sweeps of evenly spaced points
- Multiple variables can be swept in a single Sampler run
 - Sampler performs the full matrix of all combinations of all variables
- Expression variable blocks are still evaluated and substituted in inputs

Input requirements

- *parametric* block in input
 - Remove *perturb_geom* and/or *perturb_xs* from *parameter* block
- List variables and number of samples per variable in *parametric* block
 - *variables= ... end*
 - *n_samples= ... end*
 - Total number of cases generated is the product of all the *n_samples* inputs given full matrix parametric behavior

Variable blocks for parametric variables

- Distribution must be set to uniform
- Minimum and maximum set range of the variable for the study
- Inputs are equally spaced between min and max values:
 - $n_samples=1$ uses just the minimum
 - $n_samples=2$ uses the minimum and maximum
 - $n_samples \geq 3$ creates minimum, maximum, and $(n-2)$ equally spaced additional inputs

Example

```
=sampler
'
read parameters
  run_cases=no
  library="v7.1-252n"
end parameters
'
read parametric
  variables= fuel_r refl_r end
  n_samples= 5 10 end
end parametric
'
read case[hmf_004]
  import="/home/wm4/scale_training/TSU-Sampl_Fall17/Sampler_siren/HMF-004-keno.inp"
end case
'=====
'
' sample fuel radius with assumed tolerance of +/- 0.5 mm
'
read variable[fuel_r]
  distribution=uniform
  minimum=6.5037 value=6.5537 maximum=6.6037
  siren="/csas5/geometry/global_unit/sphere[1]/dimensions/r"
  cases= hmf_004 end
end variable

' sample water reflector radius with assumed tolerance of +/- 1 cm
'
read variable[refl_r]
  distribution=uniform
  minimum=32.471
  value=33.471
  maximum=34.471
  siren="/csas5/geometry/global_unit/sphere[2]/dimensions/r"
  cases= hmf_004 end
end variable
'=====
'
read response[keff]
  type = grep
  regexp = ":kenova.keff:"
  eregexp = ":kenova.keff:"
end response

end
```

Parametric output

- Sampler provides:
 - Table of variables and responses for all cases
 - Minimum of parametric study
 - Maximum of parametric study
- Value for each variable is provided with the minimum and maximum values

Minimum and maximum value edits for example

```
*****
*
*                               Parametric study minimum                               *
*****

-----+-----
response |          min      fuel_r      refl_r
-----+-----
Case hmf_004, response keff |  9.92900e-01 6.52870e+00 3.40266e+01

*****
*
*                               Parametric study maximum                               *
*****

-----+-----
response |          max      fuel_r      refl_r
-----+-----
Case hmf_004, response keff |  1.00810e+00 6.60370e+00 3.44710e+01
```

Parametric studies

- Workshop 3



Objectives

- Develop Sampler input for parametric studies from KENO input provided
- Run a (small) series of calculations to get a rough estimate of the max/min k_{eff} resulting from exploration of the parametric space

Problems

- Choose the system that is most relevant to you:
 1. Critical radius for $^{239}\text{Pu}/\text{H}_2\text{O}$ mixture
 - Pu239-h2o_sphere.inp provided as base input
 2. Optimum pitch for PWR fuel rods
 - 3d_pincell.inp provided as base input

Critical mass of ^{239}Pu

- KENO input is Pu239-h2o_sphere.inp
- Use parametric block to find the critical radius for the 20% Pu and 80% H_2O mixture
- If you have more time, look at other $^{239}\text{Pu}/\text{H}_2\text{O}$ fractions

Fuel rod pitch optimization

- KENO input is 3d_pincell.inp
- Find the pitch that results in the maximum k_{eff} value
- If you have more time, look at other rod ODs

Notes/cautions

- Choose the precision you'd like, keeping in mind the stochastic uncertainty of the KENO calculations: don't chase precision
 - Limited time available in this workshop
- Select a range and number of points
 - Wider range will require more calculations for the same level of precision in the final answer

Parametric studies

- Workshop 3 solutions



My results

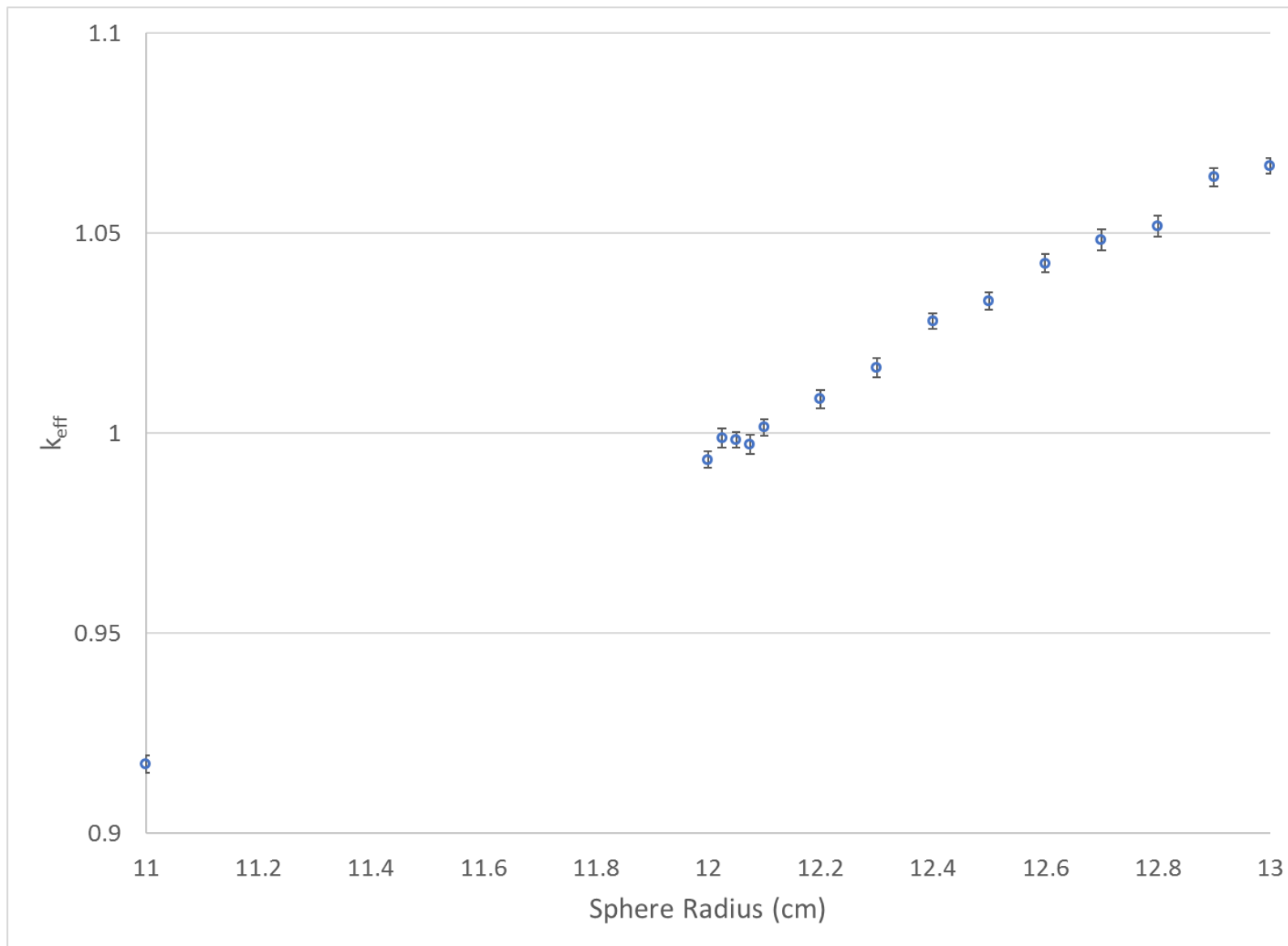
Problem	Solution
Critical radius of $^{239}\text{Pu}/\text{H}_2\text{O}$ mixture	12.03 cm
Pin cell optimum pitch	1.42 cm

Critical (k=1) sphere radius

- Series of calculations spanning a wide range, then smaller ranges in more detail at each step
 - 1 cm steps, 0.1 cm steps, 0.025 cm steps
- Results shown here and in plot on next slide
 - Note lower uncertainty KENO calculations would be needed to have confidence in results with more precision than about ± 0.05 cm
- Input blocks on subsequent slide

radius (cm)	keff	sigma
10	0.8232	0.0022
11	0.9173	0.0021
12	0.9934	0.002
12.025	0.9988	0.0024
12.050	0.9983	0.0019
12.075	0.9973	0.0024
12.1	1.0015	0.0021
12.2	1.0086	0.0023
12.3	1.0165	0.0024
12.4	1.028	0.002
12.5	1.0331	0.0021
12.6	1.0425	0.0023
12.7	1.0483	0.0026
12.8	1.0517	0.0026
12.9	1.064	0.0023

Plot of k_{eff} vs. radius



Input blocks

```
read parametric
  variables= radius end
  n_samples= 11 end
end parametric
```

```
'
' sweep from 5 to 15 by 1 (11 points)
'
read variable[radius]
  distribution=uniform
  minimum=5 maximum=15 value=10
  siren="/csas5/geometry/global_unit/sphere/dimensions/r"
  cases= PuH2O end
end variable
```

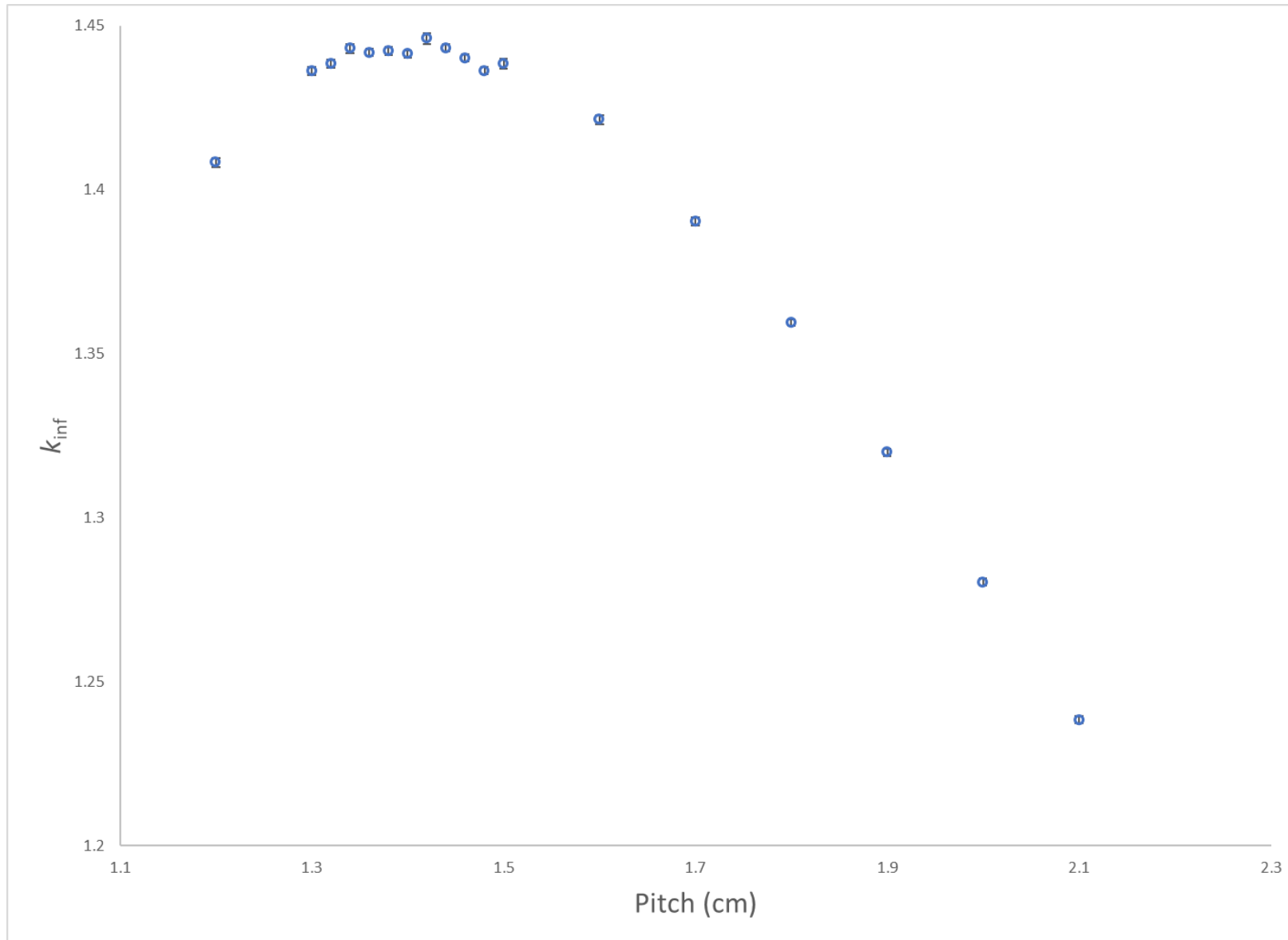
```
'
' sweep from 12 to 13 by 0.1 (11 points)
'
read variable[radius]
  distribution=uniform
  minimum=12 maximum=13 value=12.5
  siren="/csas5/geometry/global_unit/sphere/dimensions/r"
  cases= PuH2O end
end variable
```

Pin cell optimization

- First, I did a coarse sweep with 0.1 cm steps
- Then I followed up with a finer sweep between 1.3 and 1.5 cm by 0.02 cm steps
- Results shown here and in plot on next slide
 - Note lower uncertainty KENO calculations would be needed to have confidence in results with more precision than about ± 0.1 cm
- Input blocks on subsequent slide

pitch (cm)	keff	sigma
1.2	1.4083	0.0013
1.3	1.4363	0.0013
1.32	1.4385	0.0013
1.34	1.4431	0.0014
1.36	1.4419	0.0012
1.38	1.4424	0.0013
1.40	1.4414	0.0012
1.42	1.4461	0.0016
1.44	1.4433	0.0012
1.46	1.4402	0.0012
1.48	1.4363	0.0011
1.5	1.4384	0.0016
1.6	1.4214	0.0014
1.7	1.3904	0.0012
1.8	1.3595	0.0010
1.9	1.3199	0.0012
2	1.2804	0.0012
2.1	1.2384	0.0012

Plot of k_{inf} vs. pitch



Input blocks

```
read parametric
  variables= pitch end
  n_samples= 10 end
end parametric
'
' sweep pitch from 1.2 to 2.1 by 0.1 (10 points)
'
read variable[pitch]
  distribution=uniform
  minimum=1.2 value=1.26 maximum=2.1
  cases= pincell end
end variable
```

First

```
'
' detailed sweep of pitch from 1.3 to 1.5 by 0.02 (11 points)
'
read variable[pitch]
  distribution=uniform
  minimum=1.3 value=1.26 maximum=1.5
  cases= pincell end
end variable
```

Second

```
read parametric
  variables= pitch end
  n_samples= 11 end
end parametric
```

Placeholders in KENO input

```
read celldata
  latticecell squarepitch fuelr=0.39212 1 cladr=0.4572 2 pitch=#{pitch} 3 end
end celldata
```

```
global unit 1
  cylinder 1 1 0.39212 365.76 0 origin 0.63 0.63
  cylinder 2 1 0.4572 365.76 0 origin 0.63 0.63
  cuboid 3 1 #{pitch} 0 #{pitch} 0 365.76 0
end geom
```

Questions?

