Definition of K-eff

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Introduction

It might come as a surprise to readers to be told that the definition of K-eff and the terms that contribute to it (production, absorption, and leakage) are not the same in all codes. **In particular, it is important for readers to understand that MCNP and TART do not use the same definitions. The differences are due to how each code treats (n,2n), (n,3n), etc. Either the MCNP or TART definitions can be used and both have been used for many years; there is nothing intrinsically wrong with either.** The difference between their definitions only becomes important when we wish to compare results from more than one code. To compare results we must adopt one standard set of definitions to interpret the results from all codes. In my reports results are presented based on TART's definitions; however, I should mention that for the convenience of code users, the output report for each TART run includes results using both TART and MCNP definitions. With that said, let me derive the definitions used by each code.

The first point to stress is that nothing I write here is new; the ideas presented here have been known for many years, but we repeat these ideas here because definitions can effect the interpretation of the results presented for any calculation. When we discuss the sources of differences between results from a variety of computer codes, one thing we must consider is that all codes do not use exactly the same definitions. Even if two codes do the same calculation and neutron history by history get the same answers, how these results are interpreted using different definitions can impact even simple integral quantities, such as K-eff.

Time Independent (Static) Formulation

For time independent codes there is what seems like a very simple textbook definition that can be used to define K-eff. It is the ratio of the number of neutrons produced in one generation to the number produced in the preceding generation; sounds simple and unique. Unfortunately, all textbooks and codes do not use the same definition of a "generation" and/or neutrons "produced". The time independent problem is a classic eigenvalue problem that can be written in several different forms – in all of these forms we have the same left hand side of the equation, A N = $\Omega * \nabla N + \Sigma t * N$

Where A N can be defined as,

1) A N = λ T N
2) A N = λ F N + O N
3) A N = λ [F N + M N] + S N

In all case the eigenvalue λ = 1/K. Here in 1) T N is the Total (T) transfer; in 2) F N is the fission transfer, and O N is all other transfer [(n,2n)+(n,3n)+…]; in 3) F N is the fission, M N is multiple neutron transfer, e.g., (n,2n), and S N is one neutron transfer, e.g., scatter. The actual value of the calculated eigenvalue, λ, depends on which form is used, and therefore so does K. Many textbooks on particle transport will use the simplest form 1), where all secondary particles are multiplied by λ (1/K); I do not know of any computer codes that use this form, i.e./, this form is used in textbooks only because of its mathematical simplicity. The difference between 2) and 3) is how multiple neutron transfer, e.g., (n,2n), is handled. Most textbooks assume all neutron multiplication is only due to fission and use form 2). This is for historical reasons dating back many years ago to when the original transport codes were written (actually diffusion, then Sn). These codes did not include (n, 2n), etc. and fission was defined by a single secondary distribution, $\chi(E,E')$. Later when (n,2n) was included it was difficult to include it similar to fission as a neutron production term, and mathematically the simplest way to include (n,2n) was as **a negative absorption** term. But this negative absorption can lead to some strange results in order to define our all important neutron balance; I'll illustrate this point below where we see **negative absorption**.

Time Dependent (Dynamic) Formulation

For time dependent codes or codes that define K-eff in terms of a balance between neutrons produced and removed this is more complicated, because fission is not the only process that can produce neutrons during a generation; there is also (n,2n), (n,3n), etc., and how codes handle these terms lead to different definition of K-eff. Below I'll explain the differences.

Starting from the time dependent, linear Boltzmann equation in general geometry,

$$\frac{1}{v}\frac{\partial N}{\partial t} + \Omega * \nabla N + \Sigma t * N = \iint (< v > \Sigma f + \Sigma scatter + 2\Sigma n{,}2n + 3\Sigma n{,}3n + ...) N d\Omega' dE'$$

Where $N(r,\Omega,E,t)$ is the neutron flux, $v * n(r,\Omega,E,t)$, $n(r,\Omega,E,t)$ is the neutron density, v is the neutron speed, Σt is the macroscopic total cross section, $< v >$ is the average number of neutrons emitted per fission, Σf, $\Sigma scatter$, $\Sigma n{,}2n$, $\Sigma n{,}3n$, etc., are the macroscopic cross sections for each type of event. For simplicity I will use neutron density $n(r,\Omega,E,t)$ in the following, Integrate over all space, energy, and direction

$$\frac{\partial n}{\partial t} + [\,L * v * n\,] + [\,\Sigma t * v * n\,] = [(< \nu > \Sigma f + \Sigma scatter + 2\Sigma n{,}2n + 3\Sigma n{,}3n + ...)v * n]$$

Collecting terms together we find a simple equation defining the time dependent behavior of the neutron density in the system,

$$\frac{\partial n}{\partial t} = \alpha * n$$

$$\alpha = [(< \nu > \Sigma f + \Sigma scatter + 2\Sigma n{,}2n + 3\Sigma n{,}3n + ...)v] - [L * v] - [\Sigma t * v]$$

= [Production rate] – [Removal Rate]

The **time constant** (α) is a physical observable and as such has a unique value that we can determine or measure; so that its definition is unique and not subject to how it is defined. In contrast, the non-uniqueless of K-eff and related terms is because exactly the same terms appear in this definition of α as positive and negative terms that we can completely cancel (scatter), or are simply related terms that we can partially cancel (n,2n).

I will divide the total cross section by events according to how many neutrons result from each type of event: **none** – capture, (n,p), (n,a), etc., **one** – scatter, (n,np), (n,na), etc., **more than one** – fission, (n,2n), (n,3n), etc.. All of those events that result in one neutron do not directly effect the neutron balance of the system (they effect it indirectly through the leakage), and appear in exactly the same form in this definition as positive and negative terms, so that we can cancel them. Upon cancelling all scatter, and all other reactions with one neutron emitted, (n,np), (n,na), etc.,

$$\alpha = [(< \nu > \Sigma f + 2\Sigma n{,}2n + 3\Sigma n{,}3n + ...)v] - [L * v] - [(\Sigma n{,}0 + \Sigma f + \Sigma n{,}2n + \Sigma n{,}3n + ...) * v]$$

Up to this point all or least most of the codes use the same definitions. Let me stress this point: both MCNP and TART calculate roughly the same values for each of the terms in the above definition of α; there is no difference up to this point. As we will see below, the difference arises only because MCNP and TART use different definitions of neutron production and absorption.

TART defines neutron production and absorption without any further cross cancellation of terms in the above definition of α .In other words, any event that introduces additional neutrons into the system is considered production, and any event that produces neutrons also removes neutrons, etc., (n,2n) removes one neutron and produces two neutrons,

Production rate = $[(< \nu > \Sigma f + 2\Sigma n{,}2n + 3\Sigma n{,}3n + ...)v]$

Removal Rate = Leakage + Absorption = $[L * v]$ + $[(\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + ...) * v]$

Other codes, such as MCNP, change this to agree with the textbook definition of K-eff where production is only due to fission. This requires that they subtract $2\Sigma n,2n + 3\Sigma n,3n + ..$ from the TART definuition of production and removal resulting in the definitions,

Production rate = $[(< \nu > \Sigma f)v]$
Removal Rate = $[L * v]$ + $[(\Sigma n,0 + \Sigma f) * v]$ - $[(\Sigma n,2n + 2\Sigma n,3n + 3\Sigma n,4n + ...) * v]$

Note, that we still have exactly the same definition of the physically observable time constant (α), and for an exactly critical system K-eff remains unity using any of these definitions. Regardless of how they define production and removal, the codes define,

α = [Production Rate] – [Removal Rate] = [$\frac{\Pr oduction}{\operatorname{Re} moval}$ - 1]*[Removal Rate]

= [K-eff – 1]/Tr Tr = Removal Time

K-eff = $\frac{\Pr oduction}{\operatorname{Re} moval}$ Removal Time = 1/[Removal Rate]

Here we can see that even though the time constant (α) has a unque definition, K-eff and the removal time, do not; again let me stress that this is only because all codes do not define production and removal the same way. With the TART definition any event that produces more than one neutron ends a generation, and adds to the removal $\Sigma f + \Sigma n,2n + \Sigma n,3n + ...$ It also adds to the production $< \nu > \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...$ Codes that do not consider that $(n,2n),(n,3n),$ etc., end a generation (e.g., MCNP), they add nothing to production for these events and **subtract** from the removal $\Sigma n,2n + 2\Sigma n,3n + 3\Sigma n,4n + ...$

For exactly critical systems, (K-eff=1) the production and removal exactly balance regardless of which definition we use, but even in this case the individual terms, production, absorption and leakage can be quite different. I will define,

P = $[(< \nu > \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...)v]$
R = $[L * v]$ + $[(\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + ...) * v]$
M = $[(2\Sigma n,2n + 3\Sigma n,3n + ...)v]$

TART K-eff = $\frac{P}{R}$ MCNP K-eff = $\frac{P - M}{R - M}$

In this form we can see that,

Super-critical: P > R: MCNP K-eff > TART K-eff

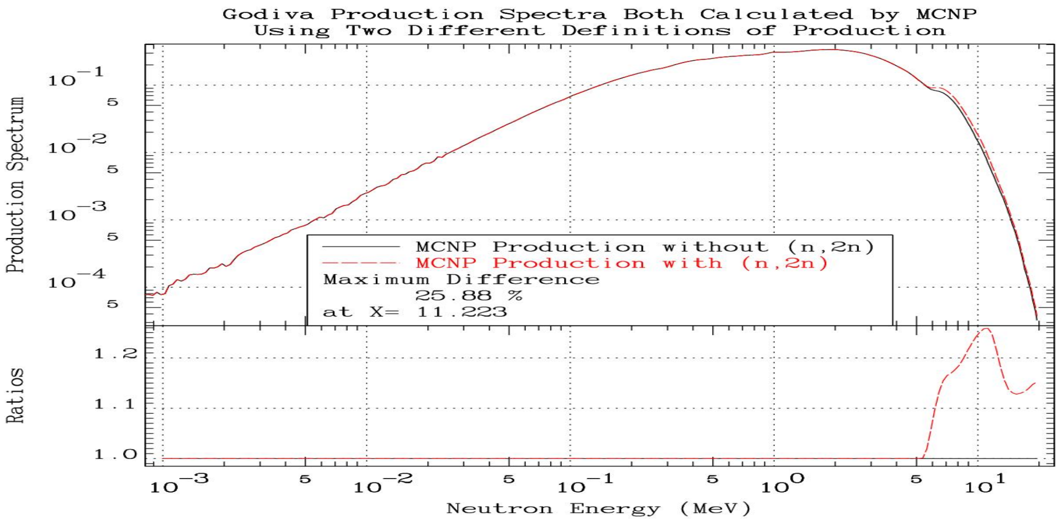
Exactly critical: P = R: MCNP K-eff = TART K-eff = 1
Sub-Critical: P < R: MCNP K-eff < TART K-eff

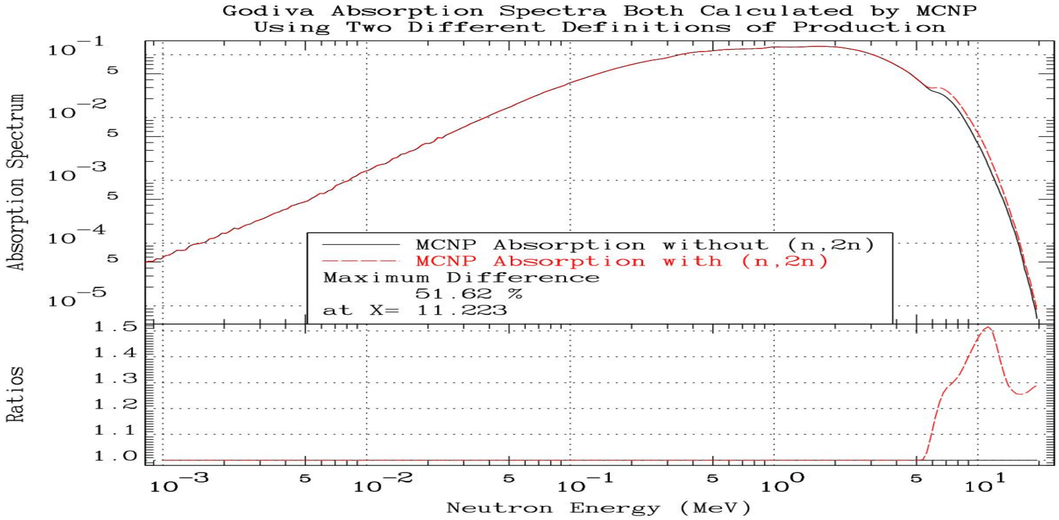
Earlier in this report we showed comparisons of energy dependent production, absorption and leakage. Even for an exactly critical system, K-eff = 1, it would have been impossible to obtain agreement when comparing results unless we used a single consistent set of definitions for production, absorption, and leakage. For example, if for production we compared the energy dependent production as defined by MCNP to the production defined by TART, we would not expect to obtain agreement, because the TART results would include the effect of (n,2n), etc., and MCMP would not. Let us stress that either MCNP or TART definitions are perfectly acceptable, but for the comparisons shown in this report we had to adopt one set of definitions; in this report I arbitrarily adopted the TART conventions to define production, absorption and leakage. The importance of using unique definitions is illustrated below using only MCNP results, but two different definitions of production and absorption.

Godiva Production and Absorption Spectra Using Two Different Definitions

In order to illustrate the importance of using unique definitions when performing comparisons, below we use MCNP Godiva results to illustrate the energy dependent production and absorption spectra using two different definitions: first MCNP's standard definition without including (n,2n), and next TART's standard definition including (n,2n). **It is important to understand that both results are based on exactly the same SINGLE MCNP calculation, and they differ only in how we interpret the MCNP results.**

What we see is that the spectra are identical up to the (n,2n) threshold; above this energy point the production and absorption spectra including (n,2n) will obviously exceed the spectra without (n,2n). **The important point to note is that had we compared MCNP results using its standard definition without including (n,2n) to TART results using its standard definition including (n,2n), we would have been mislead into thinking that the codes disagree in their transport of high energy neutrons, where in fact they agree quite well WHEN WE USE UNIQUE DEFINITIONS.**





Critical Godiva

To illustrate the difference in results due to definitions the standard TART output includes K-eff defined using both TART's definition and MCNP's definition. Below is an example portion of a TART output listing for Godiva: after tracking N neutrons to determine which lead to leakage, absorption and/or production, the results are arbitrarily normalized per neutron removed.

First, I use TART's definition, where (n,2n), (n,3n), etc., are included in absorption, and 2(n,2n), 3(n,3n), etc., are included in production. Because this is a very fast system we see that (n,2n) produces about 0.5% of the neutrons, compared to 99.5% produced by fission.

Next, I use MCNP's definition where only fission contributes to production; not (n,2n), (n,3n), etc. In this case (n,2n), etc., are treated as **negative absorption**; obviously this assumption is physically s unrealistic, but here it is merely a mathematical convenience. I haven't changed the normalization in order to maintain the same definition of Leakage (in principle this is a physical observable that could be measured directly). The removal is reduced by about 0.5%, but so is production. The net result is that in both cases we get the same value for K-eff (1.00025), even though how we define production and removal are quite different.

```
 Analog Removal and Production vs. Reaction C Number per Removed Neutron
-----------------------------------------------------------------
C Number Reaction   Removal      Production   Events
-----------------------------------------------------------------
      10 Elastic    0.00000D+00  0.00000D+00  1.64320D+00
      11 (n,n')     0.00000D+00  0.00000D+00  5.60583D-01
      12 (n,2n)     2.54982D-03  5.09963D-03  2.54982D-03
      13 (n,3n)     2.51910D-06  7.55730D-06  2.51910D-06
      14 (n,4n)     3.00000D-10  1.20000D-09  3.00000D-10
      15 Fission    3.82883D-01  9.95144D-01  3.82883D-01
      46 (n,g)      4.47771D-02  0.00000D+00  4.47771D-02
         Leakage    5.69789D-01  0.00000D+00
-----------------------------------------------------------------
         Totals     1.00000D+00  1.00025D+00  2.63400D+00
         K-eff                   1.00025D+00
-----------------------------------------------------------------
 Alternate Definition of K-eff using ONLY Fission Production
-----------------------------------------------------------------
C Number Reaction   Removal      Production
-----------------------------------------------------------------
      12 (n,2n)    -2.54982D-03  0.00000D+00
      13 (n,3n)    -5.03820D-06  0.00000D+00
      14 (n,4n)    -9.00000D-10  0.00000D+00
      15 Fission    3.82883D-01  9.95144D-01
      46 (n,g)      4.47771D-02  0.00000D+00
         Leakage    5.69789D-01  0.00000D+00
-----------------------------------------------------------------
         Totals     9.94894D-01  9.95144D-01
         K-eff                   1.00025D+00
```

HMF066-9

Now let's look at a system that contains beryllium and has many (n,2n) reactions; below are results for HMF006-9, where over 10% of the neutrons produced are due to (n,2n). As we move away from criticality the results become more sensitive to the definition we use. Now we see a difference even in K-eff: TART (0.9865) and MCNP (0.9853), for a difference of 0.0012, which exceeds the 0.1% agreement we are trying to achieve.

Note, that the difference is still quite small, near 0.1%; the important point to understand is that both MCNP and TART do the same calculations and generally get the same results. The differences we see here are based strictly on how we interpret the results – in particular, how we define production and absorption. This makes it difficult to blindly comparing results from different codes, without considering the definitions they use.

```
 Analog Removal and Production vs. Reaction C Number per Removed Neutron
-----------------------------------------------------------------
C Number Reaction   Removal      Production   Events
-----------------------------------------------------------------
      10 Elastic    0.00000D+00  0.00000D+00  8.46671D+00
      11 (n,n')     0.00000D+00  0.00000D+00  3.77274D-01
      12 (n,2n)     4.62875D-02  9.25749D-02  4.62875D-02
      15 Fission    3.51294D-01  8.94127D-01  3.51294D-01
      42 (n,t)      3.05810D-06  0.00000D+00  3.05810D-06
      45 (n,a)      3.33150D-02  0.00000D+00  3.33150D-02
      46 (n,g)      6.70535D-02  0.00000D+00  6.70535D-02
         Leakage    5.02047D-01  0.00000D+00
```

```
-----------------------------------------------------------------
         Totals      1.00000D+00  9.86702D-01  9.34193D+00
         K-eff                    9.86702D-01
-----------------------------------------------------------------
 Alternate Definition of K-eff using ONLY Fission Production
-----------------------------------------------------------------
C Number Reaction    Removal      Production
-----------------------------------------------------------------
      12 (n,2n)     -4.62875D-02  0.00000D+00
      15 Fission     3.51294D-01  8.94127D-01
      42 (n,t)       3.05810D-06  0.00000D+00
      45 (n,a)       3.33150D-02  0.00000D+00
      46 (n,g)       6.70535D-02  0.00000D+00
         Leakage     5.02047D-01  0.00000D+00
-----------------------------------------------------------------
         Totals      9.07425D-01  8.94127D-01
         K-eff                    9.85345D-01
```

HMF066-9 Sub and Super Critical

The above HMF066-9 results are what we expect for K-eff close to 1.0. Merely to illustrate differences in defined K-eff when we are further from critical, below I present results for completely hypothetical sub and super critical systems. I first decreased and then increased the density of the fuel in HMF066-9 to make it first sub critical and then super critical

Sub Critical

` Analog Removal and Production vs. Reaction C Number` **per Removed Neutron**

```
-----------------------------------------------------------------
C Number Reaction   Removal      Production   Events
-----------------------------------------------------------------
      10 Elastic    0.00000D+00  0.00000D+00  8.86549D+00
      11 (n,n')     0.00000D+00  0.00000D+00  3.01481D-01
      12 (n,2n)     5.00123D-02  1.00025D-01  5.00123D-02
      15 Fission    2.97755D-01  7.56188D-01  2.97755D-01
      40 (n,p)      4.62963D-06  0.00000D+00  4.62963D-06
      42 (n,t)      1.54321D-06  0.00000D+00  1.54321D-06
      45 (n,a)      3.63827D-02  0.00000D+00  3.63827D-02
      46 (n,g)      5.98256D-02  0.00000D+00  5.98256D-02
         Leakage    5.56019D-01  0.00000D+00
-----------------------------------------------------------------
         Totals     1.00000D+00  8.56213D-01  9.61095D+00
         K-eff                   8.56213D-01
-----------------------------------------------------------------
 Alternate Definition of K-eff using ONLY Fission Production
-----------------------------------------------------------------
C Number Reaction   Removal      Production
-----------------------------------------------------------------
      12 (n,2n)    -5.00123D-02  0.00000D+00
      15 Fission    2.97755D-01  7.56188D-01
      40 (n,p)      4.62963D-06  0.00000D+00
      42 (n,t)      1.54321D-06  0.00000D+00
      45 (n,a)      3.63827D-02  0.00000D+00
      46 (n,g)      5.98256D-02  0.00000D+00
         Leakage    5.56019D-01  0.00000D+00
-----------------------------------------------------------------
         Totals     8.99975D-01  7.56188D-01
         K-eff                   8.40232D-01
```

Super Critical

` Analog Removal and Production vs. Reaction C Number` **per Removed Neutron**

```
-----------------------------------------------------------------
C Number Reaction   Removal      Production   Events
-----------------------------------------------------------------
      10 Elastic    0.00000D+00  0.00000D+00  7.99639D+00
      11 (n,n')     0.00000D+00  0.00000D+00  4.72933D-01
      12 (n,2n)     4.23259D-02  8.46519D-02  4.23259D-02
      13 (n,3n)     1.62963D-05  4.88889D-05  1.62963D-05
      15 Fission    4.20087D-01  1.07184D+00  4.20087D-01
      40 (n,p)      2.96296D-06  0.00000D+00  2.96296D-06
      42 (n,t)      1.18519D-05  0.00000D+00  1.18519D-05
      45 (n,a)      2.96622D-02  0.00000D+00  2.96622D-02
      46 (n,g)      7.59896D-02  0.00000D+00  7.59896D-02
         Leakage    4.31908D-01  0.00000D+00
-----------------------------------------------------------------
         Totals     1.00000D+00  1.15654D+00  9.03742D+00
         K-eff                   1.15654D+00
-----------------------------------------------------------------
 Alternate Definition of K-eff using ONLY Fission Production
-----------------------------------------------------------------
C Number Reaction   Removal      Production
-----------------------------------------------------------------
```

```
       12 (n,2n)    -4.23259D-02  0.00000D+00
       13 (n,3n)    -3.25926D-05  0.00000D+00
       15 Fission    4.20087D-01  1.07184D+00
       40 (n,p)      2.96296D-06  0.00000D+00
       42 (n,t)      1.18519D-05  0.00000D+00
       45 (n,a)      2.96622D-02  0.00000D+00
       46 (n,g)      7.59896D-02  0.00000D+00
          Leakage    4.31908D-01  0.00000D+00
 -----------------------------------------------------------------
          Totals     9.15304D-01  1.07184D+00
          K-eff                   1.17102D+00
```

Compared to HMF066-9 close to critical, now we see larger differences:
Sub-critical: TART (0.8562) and MCNP (0.8402); 0.0160 difference
Super-critical: TART (1.1565) and MCNP (1.1712); 0.0147 difference

Here the differences are well over 1%, at least an order of magnitude more than the 0.1% agreement we are hoping to achieve. Note that these differences are as predicted, where for sub-critical systems, MCNP K-eff < TART K-eff, and for super-critical systems MCNP K-eff > TART K-eff. The magnitude of the difference between the definitions of K-eff depend both on how far the system is from criticality and how much n,2n, etc., reactions occur in the system.

In these cases which value of K-eff is correct? The answer is that they both are correct, based on the definitions that TART and MCNP use.

Bottom line: With all that said, let me repeat what was said at the beginning of this section defining K-eff. MCNP and TART use different definitions of production and absorption. The differences are due to how each code treat (n,2n), (n,3n), etc. Either the MCNP or TART definitions can be used and both have been used for many years; there is nothing intrinsically wrong with either. The difference between their definitions only becomes important when we wish to compare results. To compare results we must adopt one standard set of definitions to interpret the results from all codes. For this report all of the comparison results presented here are based on TART's definitions.