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Uncertainty Analysis of RELAP5-3D©

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Abstract

As world-wide energy consumption continues to increase, so does the demand for the use of alternative energy sources, such as Nuclear Energy. Nuclear Power Plants currently supply over 370 gigawatts of electricity, and more than 60 new nuclear reactors have been commissioned by 15 different countries. The primary concern for Nuclear Power Plant operation and lisencing has been safety. The safety of the operation of Nuclear Power Plants is no simple matter- it involves the training of operators, design of the reactor, as well as equipment and design upgrades throughout the lifetime of the reactor, etc. To safely design, operate, and understand nuclear power plants, industry and government alike have relied upon the use of best-estimate simulation codes, which allow for an accurate model of any given plant to be created with well-defined margins of safety. The most widely used of these best-estimate simulation codes in the Nuclear Power industry is RELAP5-3D. Our project focused on improving the modeling capabilities of RELAP5-3D by developing uncertainty estimates for its calculations. This work involved analyzing high, medium, and low ranked phenomena from an INL PIRT on a small break Loss-Of-Coolant Accident as well as an analysis of a large break Loss-Of-Coolant Accident. Statistical analyses were performed using correlation coefficients. To perform the studies, computer programs were written that modify a template RELAP5-3D input deck to produce one deck for each combination of key input parameters. Python scripting enabled the running of the generated input files with RELAP5-3D on INL's massively parallel cluster system. Data from the studies was collected and analyzed with SAS. Summaries of the results of our studies are presented.

Table of Contents

1 Nomenclature[1]

Accronym	Definition
ADS	Automatic Depressurization System
ALWR	Advanced Light-Water Reactor
AP600	Advanced Passive 600 MWe Reactor
CMT	Core Makeup Tank
ECCS	Emergency Core Coolant System
INL	Idaho National Laboratory
IRWST	In-containment Refueling Water Storage Tank
LBLOCA	Large Break Loss-of-Coolant Accident
LOCA	Loss-of-Coolant Accident
MSLB	Main Steam Line Break
NPP	Nuclear Power Plant
NRC	United States Nuclear Regulatory Commission [1]
PIRT	Phenomena Identification and Ranking Table
PPMCC	Pearson Product Moment Correlation Coefficient
PRHR	Passive Residual Heat Removal
PWR	Pressurized Water Reactor
SBLOCA	Small Break Loss-of-Coolant Accident
SG	Steam Generator
$\hat{\rho}$	The estimated value of PPMCC
$\hat{\mathfrak{r}}_s$	The estimated value of Spearman's rho
$\hat{\tau}$	The estimated value of Kendall's tau

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[1]Also referred to as USNRC

2   Motiviation

As scientists, we wish to confidently provide the answer to any question quantitatively. However, every measured value has uncertainty attached to it and thus any answer we provide must include uncertainty. Uncertainty in measurement is not the only uncertainty we must concern ourselves with. For any system we construct, outside factors will play some role within our calculations and findings, and therefore additional uncertainties must be accounted for in any solutions we provide.

In practice it is not reasonable to assume that we could quantify all uncertainties for a particular solution. Even if it were possible to quantify all possible solutions, combining all the uncertainties together could cause our data to lose significance, i.e. to become "washed out" in terms of significance. Therefore we must utilize practices that limit the number of uncertainties we consider for any particular problem. This is where the studies of Statistical Uncertainty Analysis and Sensitivity Analysis have resulted from.[8]

Uncertainty (and Sensitivity) Analysis continue to be vitally important to Nuclear Power Plants (NPPs), as well as many other fields. For NPPs in particular, the fields of uncertainty and sensitivity analysis are vitally important, as margins of safety for plant operation are a critical aspect of licensing and plant operation.

In 1988, the USNRC (United States Nuclear Regulatory Commission) issued a revision to the emergency core coolant system (ECCS) which allows for the use of best estimate plus uncertainty methods in safety analysis of LWRs (Light Water Reactors). In support of this licensing revision, the code scaling, applicability and uncertainty (CSAU) methodology was developed. As a part of that methodology, the Phenomena Identification and Ranking Table (PIRT) was developed.[14]

The PIRT process is a structured and facilitated elicitation process in which experts are

asked to rank various phenomena pertaining to a particular scenario. The phenomena are typically classified as "high", "medium", or "low".[6] The PIRT process of today also typically includes the utilization of best-estimate codes to assist in the ranking process of phenomena.

We wish to find a way to mathematically evaluate the accuracy of PIRTs, and to provide insight to validate and/or to make suggested changes to a given PIRT.

To do this, we utilized a RELAP5-3D input deck and a corresponding PIRT to determine variables of interest. Using those, we were able to create a variable specification file (spec file), as well as a template input file. We designed a program which was able to take the template input file and a specification file for the study and generate more specification files which would allow the study to be broken into sets. Then each set was run individually on the INL's supercomputer cluster (using a Python script), where up to 1,737 input files were created using our program, and run with a RELAP5-3D executable. The data was collected using the python script, and then a statistical analysis was conducted. A depiction of this process can be seen in Figure 1.
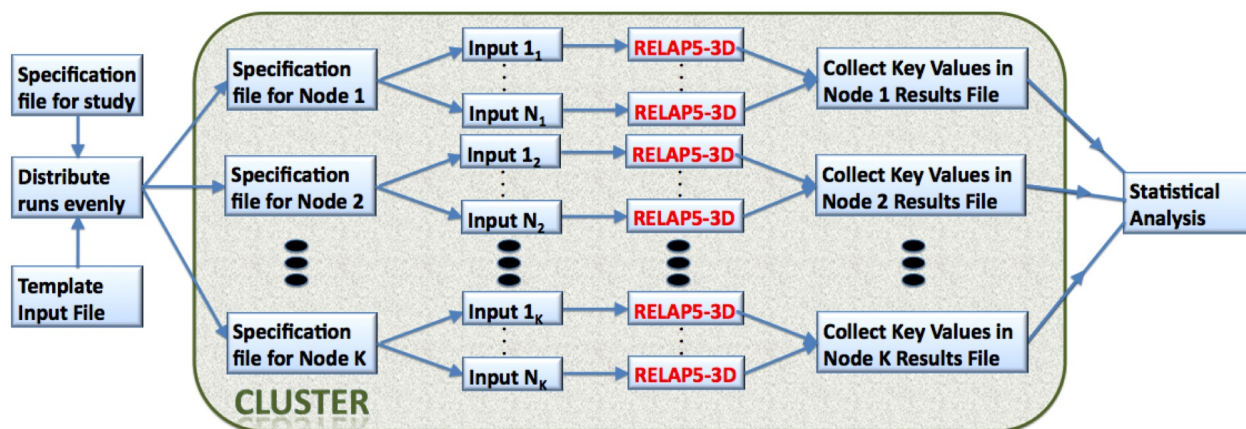
Figure 1: Algorithmic Design

We will begin by listing general statistical definitions in Section 3.1 on Page 8, defining project specific definitions in Section 3.2 on Page 10, and then discussing Coefficients of Correlation in Section 4 on Page 11. We will discuss general properties of correlation coefficients in Section 4.1 on Page 11, and discuss three types of correlation coefficients in Sections 4.2, 4.3, and 4.4 on Pages 14, 15, and 16. The relationship between the three is discussed in Section 4.5 on Page 19. We then discuss our experiments in Section 5 on Page 20. We will conclude by discussing our results in Section 6 on Page 35, summarizing our findings and discussing future work following from this project in Section 7 on Page 37.

3 Standard Formulas

3.1 General Definitions

For a general closed non-degenerate interval, $[c, d]$, with n points equally spaced within the interval (i.e. uniformly distributed), the increment size of the interval, ξ, is $\xi = \dfrac{d - c}{n - 1}$.

The probability that a sample point x will occur is the proportion of ocurrences of the sample point in a long series of experiments, and is denoted by $P(x)$. $P(x) \in [0, 1]$.

The probability density function (PDF) of a continuous random variable X, denoted by $f(x)$, is defined such that $\int_{-\infty}^{\infty} f(x)dx = 1$. The probability that an observation lies between x_1 and x_2 is defined as: $\mathrm{P}(x_1 < X < x_2) = \int_{x_1}^{x_2} f(x)dx$. The mean ($\mu_x$) or expected value $E[X]$ of the continuous random variable X, is $E[X] = \int_{-\infty}^{\infty} xf(x)dx$.

Other expectations are mathematically useful and important. We may define expecation more generally for $g(X)$, a function of the continuous random variable X, by:

$$E[g(X)] = \int_{-\infty}^{\infty} g(x)f(x)dx.$$

The variance of the continuous random variable X, where $\mu_x = E[X]$ is constant, is defined as:

$$\text{variance}(X) = \sigma_x = E[(X - \mu_x)^2] = \int_{-\infty}^{\infty}(x - \mu_x)^2 f(x)dx = E[X^2] - \{\mu_x\}^2.$$

The covariance of two random variables, X and Y with PDF $f(x,y)$, is defined as:

$$\text{Cov}(X,Y) = E[(X - \mu_x)(Y - \mu_y)] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(X - \mu_x)(Y - \mu_y)f(x,y)dydx =$$
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}xyf(x,y)dxdy - \mu_x E[X] - \mu_y E[Y] + \mu_x\mu_y = E[XY] - \mu_X\mu_Y$$

Let X be a random variable with n data points. Let each point be denoted by x_i for $i = 1, 2, ..., n$. (i.e. the data points are $x_1, x_2, ..., x_n$.)

The sample mean of X, $\hat{\mu}_x$, is defined as[2]:

$$\hat{\mu}_x = \frac{1}{n}\sum_{i=1}^{n}x_i.\text{[2, p 39,81-82,87,106-113]}$$

The sample variance of X, $\hat{\sigma}^2$, where $\tilde{s}^2$ is an unbiased estimate of $\hat{\sigma}^2$, is defined as:

$$\hat{\sigma}_x^2 = E[\tilde{s}^2] = \frac{\sum_{i=1}^{n}\left(x_i - \mu_x\right)^2}{n - 1} = \frac{\sum_{i=1}^{n}\left(x_i\right)^2 - \frac{1}{n}\left(\sum_{i=1}^{n}x_i\right)^2}{n - 1}.\text{[11, p. 11]}$$

The sample covariance of two random variables, X, and Y, each with n data points, where each point of X is denoted by x_i and each point of Y is denoted by y_i for $i = 1, 2, ..., n$, is

$$\widehat{\text{Cov}}(X,Y) = \frac{1}{n-1}\sum_{i=1}^{n}n\left[(x_i - \hat{\mu}_x)(y_i - \hat{\mu}_y)\right].$$

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[2] $\hat{\mu}_x$ is also denoted $\bar{x}$

3.2 Project Specific Definitions

In our input modification program, we are given a base file name, the number of variables, the number of sets the study will be divided into, the number of groups of variables,[3] as well as a list of variables and some basic variable information. The variable information includes the minimum and maximum values of the interval over which the variable ranges, the number of points within the interval that the variable will have (i.e. sample size), the standard deviation of the variable, the type of probability distribution the points will have within the interval (currently only the uniform is available in our program), and the group number of the variable.

For a specific variable, v, with n points, a minimum of a, and a maximum of b (where $a < b$), for which the points are distributed uniformly throughout the interval, the following formulas follow from the general definitions.

$$\xi_v = \frac{b-a}{n-1}$$

$$\hat{\mu}_v = \frac{b-a}{2}$$

$$\hat{\sigma}_v = \frac{1}{n}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left[a + \xi_v(i-1) - \hat{\mu}_v\right]^2} = \frac{1}{n}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left[a + \frac{b-a}{n-1}(i-1) - \frac{b-a}{2}\right]^2}$$

$$= \frac{1}{2n(n-1)}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left[3an - a - bn - b - 2ai + 2bi\right]^2}$$

$$\tag{1}$$

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[3]In some cases, groups of variables may need to be changed simultaneously in input file generation, and in those cases, groups are needed. In the case where a set of variables needs to be simultaneously changed all of those variables will be in one group, and in the case where only one variable needs to be changed it will be placed in its own group. For instance, in the LOFT study discussed later in the paper, variables 1-24 represent peaking factor and are in group one, variable 25 represents fuel clad gap width and is in group 2, variables 26-43 represent fuel thermal conductivityand belong to group 3, etc.

4 Coefficients of Correlation

Let X and Y be two random variables with a bivariate probability distribution.

The covariance of X and Y, denoted by $\text{Cov}(X, Y)$, is a measure of the amount of association (or, equivalently, correspondence) and the direction of association between X and Y.

The most important measure of the degree of correlation between two variables is the correlation coefficient. It standardizes the covariance in such a way as to eliminate the dependency that covariance has on the scale of measurement for the data set. [2, 187]

4.1 General Properties of Correlation Coefficients

A correlation coefficient is said to measure the strength of the relationship between variables. It is not an inferential statistical test. Rather, it is a descriptive statistical measure that depicts the strength of the relationship between two or more variables.

Let ζ denote a correlation coefficient of X and Y.

ζ should satisfy four key criteria.[3]

1. $\zeta \in [-1, 1]$

2. If the larger (smaller) values of X tend to be paired with the larger (smaller) values of $Y \Rightarrow \zeta > 0$, $\zeta \to +1$ if the correlation is strong. $\Rightarrow \exists$ a positive correlation between X and Y.

3. If the larger (smaller) values of X tend to be paired with the smaller (larger) values of Y, $\Rightarrow \zeta < 0$ and $\zeta \to -1$ if the correlation is strong. $\Rightarrow \exists$ a negative correlation between X and Y.

4. If the values of X tend to be randomly paired with the values of $Y \Rightarrow \zeta \to 0$. [4] When $\zeta \approx 0, \Rightarrow X$ and Y are uncorrelated (or, equivalently have no correlation, or zero correlation.)

Correlational information does not provide any conclusions regarding cause and effect, rather it indicates the degree of statistical relationship between two variables. [11, p 72]

The absolute value of ζ, $|\zeta|$, indicates the strength of the relationship between X and Y. As $|\zeta| \to 1$, the stronger the relationship between X and Y, and the more accurately a researcher can predict the value of y_i given x_i. As $|\zeta| \to 0$, the weaker the relationship between X and Y, and the less accurately a researcher can predict a particular y_i given x_i. When $\zeta = 0$, the relationship between X and Y cannot be predicted as ζ is no more accurate than a prediction based purely upon chance.[11, p 945-946]

The sign of ζ indicates the direction of the relationship between X and Y. $\zeta > 0$ indicates a **direct** relationship and $\zeta < 0$ indicates an **inverse** relationship.

Some general guidelines for the interpretation of ζ are:

- $\zeta \in [0.7, 1] \Rightarrow$ strong direct relationship

- $\zeta \in [0.3, 0.69] \Rightarrow$ moderate direct relationship

- $\zeta \in [0.01, 0.29] \Rightarrow$ weak direct relationship

- $\zeta \approx 0 \Rightarrow$ no consistent pattern which allows for prediction of one variable's values based upon knowledge of the other variable's values

- $\zeta \in [-0.29, -0.01] \Rightarrow$ weak indirect relationship

- $\zeta \in [-0.69, -0.3] \Rightarrow$ moderate indirect relationship

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[4] $\zeta \approx 0$ when X and Y are independent. $\zeta = 0 \nRightarrow X$ and Y are independent

- $\zeta \in [-1, -0.7] \Rightarrow$ strong indirect relationship. [11, p 72]

This allows us to make a fairly intuitive comparison of the strength of a correlation coefficient to a PIRT ranking: $|\zeta| \in [0.7, 1] \Rightarrow$ 'high', $|\zeta| \in [0.3, 0.7) \Rightarrow$ "medium', and $|\zeta| \in [0, 0.3)$ 'low'. We use this in our AP600 and LOFT studies, the results of which are discussed in Section 6 on Page 35

As with any statistical computation, it is important to determine the significance of the calculation, or in other words, it is crucial that we determine whether the correlation coefficient that we've computed is statistically significant. To determine whether the correlation coefficient is significant, it is common practice to perform inferential statistical tests to evaluate one or more hypothesis concerning the correlation coefficient. [11, p 946] In our studies, we utilized the p-value, sometimes referred to as a prob value or the associated probability or the significance probability[4, p. 18-19], as the inferential statistical test to evaluate the statistical significance of the correlation coefficient. We considered a p-value ≤ 0.05 to indicate statistical significance of the correlation coefficient. The null hypothesis, H_o, is: $H_o : \zeta = 0$, p-value $\leq 0.05 \Rightarrow$ significant evidence that there is correlation between our two variables. On the other hand, for the same H_o if the p-value $> 0.05 \Rightarrow$ we fail to reject the null hypothesis, i.e. we do not have sufficient evidence that the two variables are correlated. In our studies, if the p-value was too large, we were unable to make any conclusions about that phenomena based on its correlation coefficient.

There are many different methods of calculating correlation coefficients. The three we explore (Pearson, Spearman, and Kendall) are the most frequently used.

4.2 Pearson's Product Moment Correlation Coefficient

The Pearson Product Moment Correlation, denoted by ρ, is a measure of the **linear** relationship between X and Y. It is defined as: $\rho(X,Y) = \dfrac{\text{Cov}(X,Y)}{\sigma_X \sigma_Y}$. It is a correlation coefficient (and thus meets all four criteria specified in the section above.) In the bivariate normal case, $\rho(X,Y) = 0 \Rightarrow$ independence of X and Y.

The Pearson Product Moment Correlation Coefficient is the most commonly used measure of correlation.[11, p 71]

ρ is invariant under positive linear transformations of the random variables but it is not invariant under all order-preserving transformations, and requires that the two variables have a bivariate normal distribution.[11, p. 947] If X and Y are not approximately normally distributed, then another correlation coefficient should be used.

The most commonly evaluated hypothesis for the PPMCC is: in the population represented by the sample, the two variables have no correlation.[11, p 945]

The statistic computed for the PPMCC will be denoted by $\hat{\rho}$.

The coefficient of determination is $\hat{\rho}^2$, and it represents the proportion of variance on one variable which can be accounted for by variance on the other variable.[11, p 953]

For X and Y of sample size n, using the notation from section 3.1:

$$\hat{\rho} = \frac{\sum_{i=1}^{n} x_i y_i - \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sqrt{\left\{ \left[\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 \right] \left[\sum_{i=1}^{n} y_i - \frac{1}{n} \left(\sum_{i=1}^{n} y_i \right)^2 \right] \right\}}}. \quad [11, \text{p } 950].$$

We compute the p-values for the Pearson Product Moment Correlation Coefficient by treating $t = \sqrt{\dfrac{\hat{\rho}^2 (n-2)}{1 - \hat{\rho}^2}}$ as coming from a t-distribution with $n-2$ degrees of freedom.[10, p

18-19]

4.3 Spearman's Rho

Spearman was developed in 1904 and is a bivariate measure of correlation which is used with rank-order data.[11, p 1061] Spearman's is the application of PPMCC to ranked data.

Spearman's determines the degree to which a monotonic relationship exists between two variables.[11, p 1062]

The underlying null hypothesis for Spearman's Rank-order Correlation Coefficient is: in the population represented by the sample, the correlation between the ranks of the two is 0. [11, p 1063]

The sample statistic computed to estimate the value of Spearman's rho (or Spearman's r) will be dentoed by $\hat{\mathfrak{r}}_s$.

For X and Y of sample size n, using the notation from section 3.1 and letting R_{xi} denote the rank of variable x_i, and R_{yi} denote the rank of variable y_i:

$$\hat{\mathfrak{r}}_s = 1 - \frac{6 \sum_{i=1}^{n} \left(R_{xi} - R_{yi} \right)^2}{n \left(n^2 - 1 \right)}.$$

SAS computes $\hat{\mathfrak{r}}_s$ by ranking the data and using the ranks in the Pearson formula. When ties occur, the averaged ranks are used. The p-value for Spearman is computed by treating $t = \sqrt{\frac{\hat{\mathfrak{r}}_s^2(n-2)}{1-\hat{\mathfrak{r}}_s^2}}$ as coming from a t-distribution with $n-2$ degrees of freedom.[10, p 19] This is the same way the p-value was computed for Pearson, except that $\hat{\mathfrak{r}}_s$ is used in place of $\hat{\rho}$.

4.3.1 Generic Example of Computing Spearman's Rho and the Corresponding P-value

Suppose we have $n = 4$, and the following points, (x_i, y_i), within our data:

$(0.3, 1.5), (0.5, 2.5), (0.6, 2.3),$ and $(0.9, 4.6)$.

Ranking these points, (R_{xi}, R_{yi}): $(1, 1), (2, 3), (3, 2),$ and $(4, 4)$.

$$\Rightarrow \hat{r}_s = 1 - \frac{6 \left((1 - 1)^2 + (2 - 3)^2 + (3 - 2)^2 + (0 - 0)^2 \right)}{4 \left(4^2 - 1 \right)} = 0.8, \text{ and } t = \sqrt{\frac{0.8^2 \left(4 - 2 \right)}{1 - 0.8^2}} \approx$$

1.88562, and using a table of selected values $\Rightarrow$ p-value ≈ 0.9.

4.4 Kendall's Tau

Kendall's tau was developed in 1938 and is a bivariate measure of correlation used with rank-order data. The population parameter estimate is denoted by τ. The sample statistic computed to estimate the value of τ will be represented by $\hat{\tau}$.

Kendall's tau measures the degree of agreement between two sets of ranks with respect to the relative ordering of all possible pairs of subjects/objects.[11, p 1079]

For X and Y of sample size n, using the notation from section 3.1 and letting R_{xi} denote the rank of variable x_i and R_{yi} denote the rank of variable y_i.

A pair, (R_{xi}, R_{yi}) and (R_{xj}, R_{yj}) is said to be **concordant** if $(R_{xi} - R_{xj})(R_{yi} - R_{yj}) > 0$, or **discordant** if $(R_{xi} - R_{xj})(R_{yi} - R_{yj}) < 0$. Let n_c denote the number of concordant pairs of ranks and let n_d denote the number of discordant pairs in the ranks. Then $\hat{\tau}$ is defined as: $\hat{\tau} = \frac{n_c - n_d}{\left\{ \frac{n(n - 1)}{2} \right\}}$.

Let t_k denote the number of tied x values in the kth group of tied x values, u_l denote the number of tied y values in the lth group of tied y values, n denote the sample size, and define $\text{sgn}(z)$ as:

$$\text{sgn}(z) = \begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{if } z = 0. \\ -1, & \text{if } z < 0 \end{cases}$$

Let $T_0 = \frac{1}{2}n(n-1)$, $T_1 = \sum_k \frac{1}{2}t_k(t_k - 1)$, and $T_2 = \sum_l \frac{1}{2}u_l(u_l - 1)$.

Then we can define $\hat{\tau}$ as: $\hat{\tau} = \dfrac{\displaystyle\sum_{i<j}\big(\text{sgn}(x_i - x_j)\text{sgn}(y_i - y_j)\big)}{\sqrt{(T_0 - T_1)(T_0 - T_2)}}$.

Let $s = \displaystyle\sum_{i<j}\big(\text{sgn}(x_i - x_j)\text{sgn}(y_i - y_j)\big)$.

Define the variance of s, $V(s)$, as: $V(s) = \dfrac{v_0 - v_t - v_u}{18} + \dfrac{v_1}{2n(n-1)} + \dfrac{v_2}{9n(n-1)(n-2)}$,

where $v_0 = n(n-1)(2n+5)$, $v_t = \sum_k t_k(t_k - 1)(2t_k + 5)$, $v_u = \sum_l u_l(u_l - 1)(2u_l + 5)$,

$v_1 = \left(\sum_k t_k(t_k - 1)\right)\left(\sum_l u_l(u_l - 1)\right)$, and $v_2 = \left(\sum_k t_k(t_k - 1)(t_k - 2)\right)\left(\sum_l u_l(u_l - 1)(u_l - 2)\right)$.

We compute the p-values by treating $\dfrac{s}{\sqrt{V(s)}}$ as coming from a standard normal distribution.[10, p. 20-21]

4.4.1 Generic Example of Computing Kendall's Tau and the Corresponding P-value

To illustrate the computation of Kendall's tau, as well as the corresponding p-value, we will utilize the same example as was used in the generic example of computing Spearman's rho and its corresponding p-value in Section 4.3.1 on Page 16.

Suppose we have $n = 4$, and the following points, (x_i, y_i), within our data:

$(0.3, 1.5), (0.5, 2.5), (0.6, 2.3),$ and $(0.9, 4.6).$

Ranking these points, (R_{xi}, R_{yi}): $(1, 1), (2, 3), (3, 2),$ and $(4, 4).$

The concordant pairs are: $(1, 1), (2, 2)$ & $(1, 1), (3, 2)$ & $(1, 1), (4, 4)$ & $(2, 3), (4, 4)$ and $(3, 2), (4, 4).$

The discordant pair is: $(2, 3), (3, 2).$

$\Rightarrow n_c = 5$ and $n_d = 1.$

$$\Rightarrow \hat{\tau} = \frac{5 - 1}{\left\{ \frac{4(4 - 1)}{2} \right\}} = \frac{2}{3}$$

If we use the second formula for $\hat{\tau}$, we get the same result.

$s = 5 - 1 = 4$, $t_k = 0$, and $u_l = 0.$

$T_0 = \frac{1}{2} \times 4 \times (4 - 1) = 6$, $T_1 = 0$, and $T_2 = 0.$

$$\Rightarrow \hat{\tau} = \frac{5 - 1}{\sqrt{(6 - 0)(6 - 0)}} = \frac{2}{3}.$$

We can now compute $V(s)$.

$v_o = 4 \times (4 - 1) \times (2 \times 4 + 5) = 156$, $v_1 = 0$, and $v_2 = 0.$

$$\Rightarrow V(s) = \frac{156 - 0 - 0}{18} = \frac{26}{3}$$

$$\Rightarrow \frac{s}{\sqrt{V(s)}} = \frac{4}{\left\{\sqrt{\frac{26}{3}}\right\}} \approx 1.35873$$

Using a table of values for the standard normal distribution, $\Rightarrow$ p-value $\approx 1 - 0.3708 = 0.6292$.

4.5 Discussion of Pearson, Spearman, and Kendall

It is recommended that for interval or ratio data in the bivariate case that the Pearson product-moment correlation coefficient be used, for ordinal or rank order data of bivariate case that Spearman's rank-order correlation coefficient or Kendall's tau be used.[11, p 117]

Pearson is a stronger correlation coefficient[5] than Spearman or Kendall, but has additional restrictions, such as the requirement of parametric data.[6] Spearman's rho is more commonly used than Kendall's tau for two primary reasons. The computations for tau tend to be more tedious than those completed when calculating rho.[7][11, p. 1080] The second reason is that when the sample is derived from a bivariate normal distribution, Spearman's rho tends to provide a reasonably good approximation of Pearson, while Kendall's tau will not. An advantage of Kendall's tau is that it has a sampling distribution that approaches normality very quickly. Spearman's rho, on the other hand, needs a fairly large sample size to employ the normal distribution to approximate the sampling distribution of rho.[11, p. 1080] As a general rule, $|\tilde{\tau}_c| < |\tilde{\mathfrak{r}}_s|$ for a set of data, and $\frac{\hat{\tau}}{\hat{\mathfrak{r}}_s} \to (0.67)^2$.[11, p. 1080][8]

In Sections 4.3.1 and 4.4.1 we had $\hat{\tau} = \frac{2}{3}$ and $\hat{\mathfrak{r}}_s = 0.8$, $\Rightarrow |\hat{\tau}| < |\hat{\mathfrak{r}}_s|$, which follows the general rule. However, $\frac{\hat{\tau}}{\hat{\mathfrak{r}}_s} \approx 0.83333 \neq (0.67)^2$, yet, it does not disprove the general rule as we just used a generic example which had a very small sample space.

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[5]'Stronger' in this case is referring to a higher degree of statistical significance.

[6]Recall, it specifically requires a bivariate distribution which is approximately normal.

[7]With the advances in computing, and the introduction of statistical software packages, this has become less of an issue.

[8]This is not the case when the value of Spearman's rho is 1 or -1. In that case, Kendall's tau will also be 1 or -1 respectively. This is the same for the case when Kendall's tau is known to be 1 or -1.

5 Experimental Information

5.1 RELAP5-3D

5.1.1 Terminology and Basic Deck Requirements[7, p. A1-1]

Term/Accronym	Definition/Description
BE	Best-Estimate
Card	an 80-character record in the input deck
Card #	the first field on the data card. It is an unsigned integer, and is used to specify the component number the card supplies information about.
Comment Card	identified by a '∗' or a '$' as the first nonblank character. Blank cards are treated as comment cards. With the exception of printing out their contents, there is no processing of comment cards.
Continuation Card	identified by a '+' as the first nonblank character on the card, may follow a data card or another continuation card. Fields on each card must be completed on that particular card (i.e. a field may not continue from one card onto the next.)
Data Card	contains varying numbers of fields that may be integer real, or alphanumeric. If a matching card number is found, the data card that appears last in the deck is the card that is used.
Input Deck	term used to describe the input files
Terminator Card	identified by a '/' or a '.' as the first nonblank chearcter. Comments may follow '/' or '.' on a particular card
Title Card	identified by an '=' sign as the first nonblank characters and contains no more than 80 characters including the '='.
Word	fields on the data card following the card number, a word is terminated by comma(s) or space(s). Numeric words must begin with a digit (0-9) or a sign (+ or -), or a decimal point.

A RELAP5-3D input deck typically consists of at least one title card, optional comment cards, data cards and a terminator card.

5.1.2 Safety Analysis of NPPs & BE Codes

To ensure safety in the reactor design, operator training, and upgrades to the Nuclear Power Plant (NPP), Best Estimate (BE) codes are frequently used to model NPPs and to analyze their safety.

A *Best Estimate* code is a system code that is capable of predicting/ modeling physical phenomenon, free of any conservatism regarding selected acceptance criteria, and able to provide a sufficiently detailed model to describe the relevant processes.[9, p. 193] RELAP5-3D is the BE code used in this study.

5.1.3 About

RELAP5-3D is a fully integrated, multi-dimensional thermal-hydraulic and kinetic modeling program. It is a BE code developed at the INL, which serves as a modeling and simulation tool to support engineering design and safety analysis of nuclear reactors. It is also used for non-nuclear fields such as fossil power plants, oil and gas pipelines, municipal steam supply systems.

5.1.4 Running RELAP5-3D

Upon performing the calculations of the input model, RELAP5-3D produces three output files: a '.p' file, a '.plt' file, and a '.r' file. The '.p' file is a printed output file, the '.plt' file is a plot file, and the '.r' file is the restart file. In our studies, we were primarily concerned with examining the printed output file. We wrote a Python script, which is described in Section 5.5 on Page 33. This script locates our desired ouput parameter value from the '.p' file, and then places that value into a parameter value file which is created with the input modification program described in Section 5.4 on Page 29.

5.2 AP600 Deck

Figure 3. AP600 Passive Containment Cooling System [13]   [5]
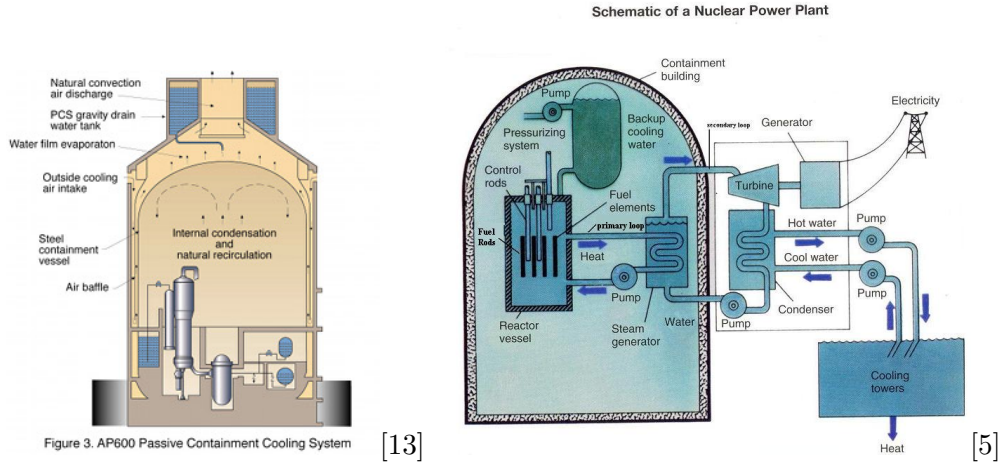
5.2.1 Background on the AP600 Nuclear Power Plant

The AP600 Nuclear Power Plant (NPP) was designed by Westinghouse as a part of the cooperative U.S. Department of Energy (DOE) and the Electric Power Research Institute (EPRI) Advance Light Water Reactor Program (ALWR). [12]

For safety, the AP600 relies on operation of passive systems. The Phenomena Identification and Ranking Table (PIRT) compiled by Burtt, et al (used in this paper, see the references section, number [1]) addresses AP600 behavior expected during small break loss-of-coolant, main steam line break, and steam generator tube rupture accidents. [1]

5.2.2 Variable Names, Representation, & Corresponding PIRT[1] Phenomena

Variable	Representing	Corresponding to (in PIRT)	PIRT Ranking
VAR1	Fission-Product Yield (i.e. decay-heat)	Core Power	High
VAR2	Roughness	Flow Resistance in the IRWST	High
VAR3	Form Loss	Flow in Accumulator (pressurized volume)	High
VAR4	Form Loss	Flow in Accumulator (pressurized volume)	High
VAR5	Area (ADS-4)	ADS Energy Release	High
VAR6	Area (Break Valve)	Mass Flow in Break[9]	High
VAR7	Area (Orifices)	Injection Line - CMT	High
VAR8	Initial Level of Pressure	Level in CMT	High
VAR9	Roughness	ADS Flow Resistance	Medium
VAR10	Roughness	ADS Flow Resistance	Medium
VAR11	Fouling Factor	PRHR (Heat Transfer between PRHR & IRWST)	Medium
VAR12	Fouling Factor	Steam Generators (Primary to Secondary Heat Transfer)	Medium
VAR13	Roughness	PRHR-Flow Resistance # 1	Low
VAR14	Roughness	PRHR-Flow Resistance #2	Low
COREMIN	Control Variable 116	Minimum Value of the Core Collapsed Liquid Level [10]	N/A

5.2.3 Studies with the AP600 Deck

Using the AP600 deck, we conducted four studies. These studies were based upon the size of break in the cold leg. Each of the 13 variables[11] had three values which were evenly distributed throughout the interval (i.e. a minimum, a mean, and a max). Variable 6 denoted the size of the break and was used to create the four different studies. To have

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[9]This was used to create the four different studies: 2 inch Break, 4 inch Break, 6 inch Break, and 8 inch Break.

[10]COREMIN is the key output parameter used in the AP600 studies

[11]i.e. VAR1-5, VAR7-14. VAR 6 was used to vary the break size.

every possible combination of variable values, this would mean creating $3^{13} = 1,594,323$ input files.

Performing even a single study with 3^{13} runs of 400 seconds would require 7,381 days on a single processor. Even utilizing the INL cluster, described in Section 5.5 on Page 33, which has 32 cores per node and 12 nodes, it would require 19 days to run the study. There are many ways to reduce the number of runs in a study. We decided to investigate the use of grouping our studies into smaller sets to reduce the number of required runs for each study. We first separated each study into two or three sets. The variables that had correlation coefficients that were ranked high or medium among the sets would then be grouped together and run again. Through experimentation, we found that separating the studies into smaller sets did not significantly affect the calculations of the relative correlation coefficients and substantially reduced the amount of time needed to run our studies.

The size of the break dictates how long the transient runs. In order to further decrease the run-time of our studies, we plotted each of the four transients (2 inch, 4 inch, 6 inch, 8 inch) to determine what the duration of the transient should be for each respective study. The duration of the transient that was selected for each study encompassed the time when the collapsed core level reached its lowest height. These plots can be seen in Figures 2, 3, 4, and 5, respectively.[12] We determined that it was effective to run the 2 inch break transient for 400 seconds, the 4 inch break transient for 200 seconds, the 6 inch break transient for 200 seconds, and the 8 inch break transient for 75 seconds.

The results from the 'top study' of each of the cold-leg break studies are presented in Section 6.1.1 on Page 35.

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[12]coremin represents the key output parameter, which is a control variable we created that takes the minimum of control variable 114 (collapsed core liquid level). Control Output() is the (Percentage of) Collapsed Core Liquid Level.
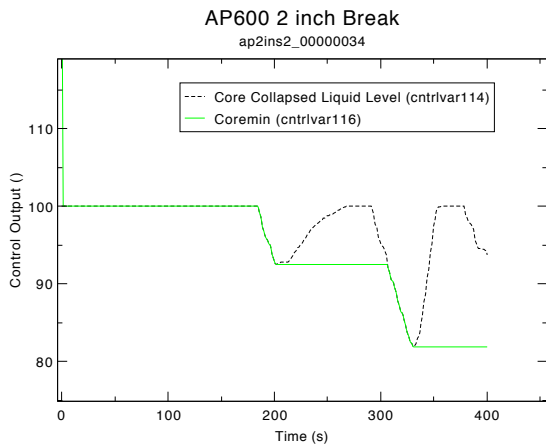
Figure 2: 2 inch Break Transient Plot   Figure 3: 4 inch Break Transient Plot
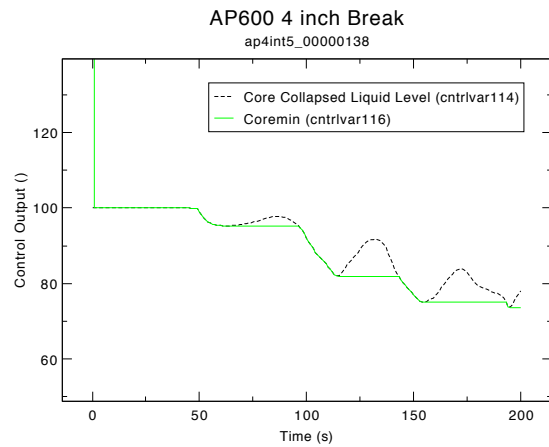
Our first study that we conducted was on a four inch break. To decrease run-time, we broke the study into two sets: the first set had only variables 1-5 and 7-8 (i.e. the PIRT-ranked 'high' variables, note that as stated previously, variable 6 is the break size and thus will not be adjusted within the 4 inch study) varying, while the other 6 variables were held at the nominal (or mean) value. The first set was $3^7 = 2,187$ input files. The second set had only variables 9-14 (i.e. the PIRT-ranked mediums and lows) varying, while the other 7 variables were held at their respective nominal values. The second set consisted of $3^6 = 729$ input files. After both sets were complete, and analyzed using SAS, we created a new study, which was based on the top 5 most correlated variables from both 4 inch studies: VAR1, VAR8, VAR11, VAR12, and VAR13. Just as before, all five variables varied between the three values while the other 8 variables were held at their respective nominal values. This created $3^5 = 243$ input files.

Our second study was on a 2 inch cold leg break. We put this study into three sections (the other variables are held at their respective nominal values): variables 1-5 varying ($2^5 = 243$ input files), variables 7-10 varying ($2^4 = 81$ input files), and variables 11-14 varying ($2^4 = 81$ input files). After all three sets were analyzed using SAS, we created a new study, based on
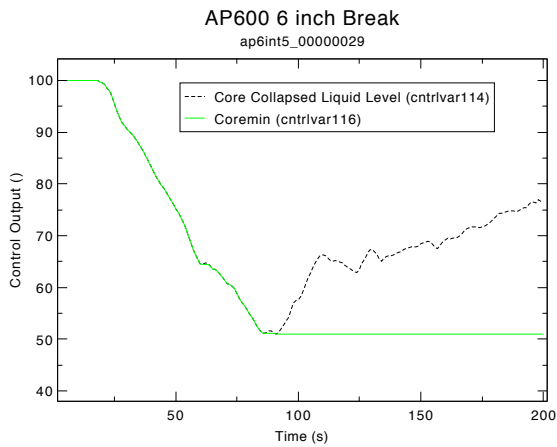
Figure 4: 6 inch Break Transient Plot
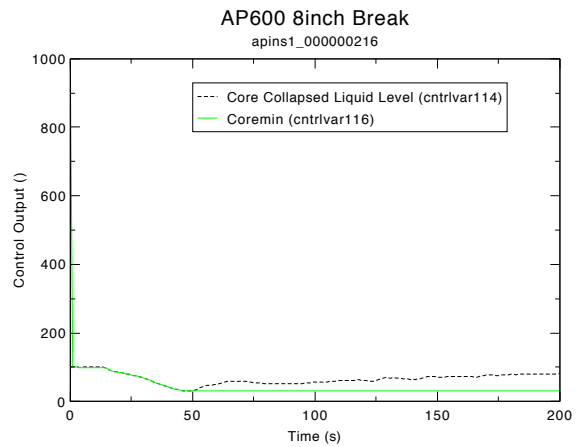
Figure 5: 8 inch Break Transient Plot

the top 4 most correlated variables from the three sets: VAR1, VAR8, VAR12, and VAR13. As with the four inch study, we varied these variables between the three variables, while the other 9 variables were held at their respective nominal values. This created $3^4 = 81$ input files.

Our third study was on a 6 inch cold leg break. We split the study into 3 sections, which were identical to the sections for the 2 inch break study. After the three sets were analyzed with SAS, a new study was created based on the top 5 most correlated variables from the three sets: VAR1, VAR7, VAR8, VAR12, and VAR13. These were varied as with the 2 inch and 4 inch break studies: the 5 variables were varied by 3 values, and the other 8 were held constant at their respective nominal values. This created $3^5 = 243$ input files.

Our final study of the AP600 deck was on an 8 inch cold leg break. As with the 2 inch and 6 inch break studies, we split the 8 inch study into the same sets. After the three sets were analyzed using SAS, a new study was created based on the top 4 most correlated variables from the three sets: VAR1, VAR8, VAR12, and VAR13, creating $3^4 = 81$ input files for this section of the study.

26

In all of the studies, there were variables which had their respective p-value > 0.05. This does not indicate that these variables were statistically insignificant, or that they were unimportant to the minimum core level. Rather, it indicates that we cannot make a conclusion regarding their correlation to the minimum core level, and that further investigation is needed for these variables.

5.3 LOFT Deck

5.3.1 Background Information on the LOFT Nuclear Power Plant

Following the 1988 revised emergency core cooling system rule for LWRs which allows the use of best estimate plus uncertainty methods in safety analysis, a study was conducted at the Idaho National Laboratory (INL) based on a cold leg large break loss of coolant accident test in the Loss of Fluid Test (LOFT) experimental facility. The LOFT facility was a 50 MW PWR that was designed to model a large break loss of coolant (LBLOCA) in a commercial pressurized water reactor (PWR). The facility was operational from the late 1970's to the mid 1980's.[15]

The input deck used in this study was the same input deck used by G.E. Wilson and C.B. Davis in their "Best Estimate Versus Conservative Model Calculations of Peak Clad Temperature: An Example Based on the LOFT Facility" paper (see reference [15].)

5.3.2 Variable Names and Corresponding Phenomena [15]

Group Number	Variable(s)	Representing
1	VAR1-VAR24	Peaking Factor (i.e. core power fractions)
2	VAR 25	Fuel Clad Gap Width
3	VAR26-VAR43	Fuel Thermal Conductivity
4	VAR 44	Clad to Coolant Heat Transfer (i.e. fouling factor)
5	VAR45-VAR46	Break Discharge Coefficient
6	VAR47-VAR51	Pump Degradation
n/a	Control Variable 234	Peak Clad Temperature [13]

5.3.3 LOFT Studies

We conducted two studies using the LOFT deck. Both studies values were selected based upon G.E. Wilson and C.B. Davis' paper. For both studies, the key output parameter in the study was Peak Clad Temperature (PCT).

In the first study, each of the six groups of variables had 3 points uniformly distributed (i.e., minimum, mean, and maximum). All groups used minimum, mean, and maximum for their three values. However, the variables within each group often had differing maxima, minima, and means. For example, in group one there were 24 different sets of minimum, mean, and maximum, yet all variables in the group needed to vary in the same way. For instance, each of the 24 variables in group one all needed to experience their respective minimum simultaneously. Likewise, each of the 24 variables in group one had to achieve their mean simultaneously. Similarly, the 24 variables all experienced their respective maxima simultaneously. There were $3^6 = 729$ input files in the first study.

In the second study, each of the six groups had 5 different values (i.e., minimum, low-mean, mean, high-mean, and maximum.) The groups of variables functioned the same way for the second study as the first study, just with additional values. In other words, for

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[13]Peak Clad Temperature is the key output parameter used in the LOFT study.

group one, the 24 variables were varied simultaneously, with each variable within the group experiencing it's particular low-mean simultaneously. Likewise, each of the 24 variables experienced its respective high-mean simultaneously. There were $5^6 = 15,625$ input files in the second study.

The results from both studies with the LOFT deck are presented in Section 6.2 on Page 36.

5.4 Input Modification Program

In order to run the AP600 study and the LOFT study, a Fortran 90$^{©}$ program was created. This program uses a marked input deck and study specification file(s) to create input files with input values varying as specified in the specification file(s).

5.4.1 Marked Input File

After an input deck[14] and the variables of interest (sometimes referred to as input parameters) as well as the key output parameter have been selected, the user must determine how these selected input parameters should vary. Once that is determined, the user should create a 'spec file' (or Specification File). Specification Files are discussed in Section 5.4.2. The base input deck should then be 'marked' by the user- this consists of locating the variables of interest (i.e. card number and word) within the deck, and then placing a '$ XXXX'[15] in place of the current value on the card in the deck.[16] This process should be undertaken simultaneously with the creation of the 'spec file' so as to avoid mistakes. [17] After the base deck is completely marked, we refer to it as the "marked input deck."

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[14]To avoid confusion, we will refer to this input deck as the base input deck.

[15]XXXX denotes the variable name of that particular input parameter

[16]In our studies, we selected 'VARX' , where $X = 1, 2, 3, ...$ to denote the various variables.

[17]There are very specific parameters for the length of character name, so care should be taken. Details of this can be found within the main program- see Appendix A for further details. Additional care should be taken when replacing values as a card may only contain 80 characters, so the user may wish to consider adjusting spaces within a given card or splitting the card (i.e. making a continuation card.) See reference [7].

5.4.2 Specification Files

The specification file(s) or 'spec file(s)', contains all of the necessary information for a given study. The first line of a spec file indicates the type of spec file it is. There are two types of spec files: (1) a Generator Specification File and (2) a Node Specification File. These are discussed in the Subsections 5.4.2(a) and 5.4.2(b) respectively. Both types of spec files contain: the base name of the files that are generated (this is also the name (without the extension) of the marked input file), the number of variables in the study, the number of nodes in the study [18], which node (or set) of this spec file corresponds to, the number of groups in the study[19], as well as variable name[20], the minimum value of the variable, maximum of the variable, standard deviation of the variable, number of variations of the variable (i.e. number of points for the variable), the distribution type of the variable, and the group number the variable belongs to[21]. A template of a spec file can be seen in Appendix B on Page 51.

4.5.2(a) Generator Specification File A "Generator Specification File" or "generator spec file" is a spec file with <u>generate</u> on the first line of the spec file. When combined with the executable produced by the input modification program, described in Section 5.4.3, it produces a specified number of *node* spec files, each of which has a different node number[22]. The node number corresponds to the INL cluster node, where each node has multiple cores. The INL cluster is discussed more in Section 5.5 on Page 33. To see an example of a

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[18]The 'number of nodes' refers to the number of studies within the study. i.e. We break each study into multiple sets (or studies) so that it is easier to run the study on the cluster. This is discussed in greater detail in Section 5.5.

[19]The 'number of groups' refers to the number of variables that vary INDEPENDENTLY within the study- i.e., in our LOFT studies, we had variables which had to vary simultaneously (dependently). For instance, variables 1-24 all varied simultaneously, variable 25 varied independently, variables 26-43 varied simultaneously, variable 44 varied independently, variables 45-46 varied simultaneously, and variables 47-51 varied simultaneously, so we had 6 groups. In the case of the AP600 studies, all 14 variables varied independently and so the number of groups was equivalent to the number of variables, 14.

[20]Note that the '$' is not written into the spec file- though it is marked that way in the marked input file. The '$' is appended within the main program, see Appendix A for more information.

[21]i.e. VAR1-24 in LOFT study are in group 1, and so a 1 is written in that variable's line.

[22]Using the notation from the template spec file in Appendix B, the specified number of spec files is #nodesInStudy, and the node number corresponds to 'currentNode'.

generator spec file, see Appendix C on Page 52.

The motivation for generating separate node spec files was cluster supercomputer limitations. Generating thousands of input files on a single processor, then moving them to the nodes where they would run ties up communication resources need for other data flow and can seriously impair performance. It is far more efficient to generate the RELAP5-3D input files on the nodes where they will run, thereby eliminating all such input file movement.

4.5.2(b) Node Specification File A "Node Specification File" or "node spec file" is a spec file with <u>run</u> on the first line of the spec file. When combined with the executable produced by the input modification program, described in Section 5.4.3, it produces the input files corresponding the particular node number of the node spec file. To see an example of a node spec file, see Appendix D.

5.4.3   Main Program

The main program, input_mod_gen.f90, is included as Appendix A on Page 40. Its purpose is to create an entire statistical study by generating input relating to a PIRT analysis. It has three purposes:

1. Interpret the "generator specification file" and create a number of "node specification files."

2. Produce all RELAP5-3D input files for a given node of the cluster supercomputer from the "node specification file" and a single RELAP5-3D input template file.

3. Handle the situation where a group of input parameters vary together (are 100% correlated).

The main program is run first to create a node specification file for each cluster node; a node may have up to 32 cores that can each run RELAP5-3D independently and simultaneously.

The creation of the node spec files from a generator spec file is done through the command line prompt:

input_mod_gen.exe -i generator_spec_file_of_my_study

This creates the corresponding node spec files and these node spec files are exported to each node along with a copy of the template input file. The main program is run on each node to produce the specific input files of the statistical study, and is run on the cluster via a Python script which is described in Section 5.5 on Page 33. The complete set of possible combinations of input values can be ordered as a set of n-tuples. The set of n-tubles is generated by a recursive algorithm and therefore works for any number of input parameters.

The ordinal number of the n-tuple that is used to generate an input file is assigned as the input file's sequence number and becomes part of its name. Concatenating its sequence number to the base name of the statistical study forms its name. All input files have a unique name, regardless of the node on which it runs. The input files are created by copying the template input file then substituting the variable values corresponding to its n-tuple into the input file for that variable's marker. Markers had the form $VAR1, $VAR2, ... VARK$. When some variables are 100% correlated, K is larger than n (the size of the n-tuples).

The values of the correlated variables are varied together. For example, if group one has 20 variables and a uniform distribution with 3 "levels" in use, namely minimum, mean, and maximum value, the group counts as one variable in the first position of the n-tuple previously discussed. The group has three levels: minimum, mean, and maximum. However, when an input file is generated, the particular "maximum value" of each variable is substituted for its marker ($VAR1 through $VAR20). Input files are created on node 3 with the following command:

32

input_mod_gen.exe -i node3_spec_file_of_my_study

. The number of input files generated is a function of the number of groups and the number of value levels within the group. For example, if group 1 has 6 variables and 3 levels, group 2 has only one variable with 8 levels, and group 3 has 9 levels, there would be $3 * 8* = 216$ combinations in the entire statistical study. The program determines the number of input files that are created by each node spec file based upon the #nodesInStudy (combSet in program) by taking the celing function of $\left\{ \dfrac{\text{\# of Input Files in Study}}{\text{\#nodesInStudy}} \right\}$. The second LOFT study had 6 groups of variables, each with 5 values for a total of 15,625 runs. Splitting these runs among 9 node spec files placed 1736 runs each on nodes 1-8 and 1737 runs on node 9.

5.5 Running on the Cluster & Python Scripting

Studies were run on one of the INL's supercomputers, Quark, which has 12 nodes. Users submit jobs, such as our statistical studies, via a batch queuing system.

Due to limited resources particularly on moving large amounts of data from the head node to computational nodes, it is much more efficient to generate the input files on the node as explained in Section 5.4.3 on Page 31.

The Python scripts are included in Appendix E on Page 53. It runs the main program on the head node of the cluster, moves the node specification file onto the cluster's computation nodes, runs RELAP5-3D in parallel on the input files, collects the output from the RELAP5-3D output files, and plaes it in a "study output file" on the line corresponding the input's n-tuple. These files are ported back to the head node and are then combined into a single "study output file."

Thereafter, SAS can be used to perform the statistical analysis.

5.6   Using SAS$^{©}$

Once all of the res files have been created, as described in Section 5.5, we copy them into the local desktop, relabeling the files' extensions as '.csv' (as opposed to '.res'), and adding an additional line to the beginning of the file which typically looks like 'runNumber,VAR1,VAR2,VAR3,....,KEYOUTPUT'. We then import each file into SAS, a statistical software package. We used the SAS package, SAS EnterpriseGuide 4.3, which offers a graphical user interface of SAS 9.2. We then combined the res files from all of the nodes into one data set, through utilization of the 'append table' feature, "tasks \ data\ append table". We then calculated the correlation coefficients using the correlation coefficient function, "tasks \ Multivariate \ Correlation Coefficient". We selected the variables as analysis variables, and correlated them with the key output parameter. The options we selected were Pearson, Hoeffding, Kendall, and Spearman, and we included the Pearson correlation options of covariances, sums of squares and crossproducts. These produced SAS reports, which are found in Appendix F. We were then able to rank the variables accordingly.

6 Results

6.1 AP600 Studies

6.1.1 AP600 Correlation Coefficient Classification

Break	High ζ	Medium ζ	Low ζ
2 inch	Core Power (PIRT High)		PRHR-Flow Resistance # 1 (PIRT Low)
4 inch	Core Power (PIRT High)		
6 inch		Core Power (PIRT High) Level in CMT (PIRT High) PRHR-Flow Resistance #1 (PIRT Low)	SG-Heat Transfer (PIRT Medium)
8 inch[23]		Core Power (PIRT High) Level in CMT (PIRT High)	SG-Heat Transfer (PIRT Medium)

6.1.2 Discussion of the Rankings of the Phenomena

All variables which were not listed in Section 6.1.1 had their respective p-value > 0.05.

In the 2 inch and 4 inch studies, the findings were as we expected based upon the PIRT recommendations. In the 6 inch and 8 inch studies, there were some surprising results. In the 6 inch study, two PIRT-ranked 'highs' had a correlation coefficient classifications of 'medium', and a PIRT-ranked 'medium' had a low correlation coefficient classification, of particular interest was that one PIRT-ranked 'low' had a medium correlation coefficient classification. In the 8 inch study, we saw a similar ranking pattern to that of the 6 inch study, with the exception being that all rankings in the 8 inch study were less than those of the PIRT, specifically, none of the rankings of the correlation coefficient classification

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[23]In the 8 inch break, the average of the correlation coefficients for the various phenomena were used. In the other studies, the three correlation coeffients were in agreement. The exact correlation coefficient values can be found in the SAS© Reports in Appendix F on Page 58.

were greater than that of the PIRT. The rankings we saw in the 6 inch study (and in the 8 inch study) which were less than or equal to the PIRT rankings do not cause too much concern as the PIRT was conservative, i.e. if the panel was unsure as to whether something should be ranked as 'high' or 'medium', they ranked it as 'high'. The result that surprised us was the phenomena in the 6 inch study which was ranked higher than the PIRT ranking in terms of correlation coefficients.

6.2   LOFT

6.2.1   LOFT Correlation Classification

Classification	Group Name(s)
High ζ	Fuel Clad Gap Width
Medium ζ	Clad to Coolant Heat Transfer & Peaking Factor
Low ζ	Break Discharge Coefficient & Fuel Thermal Conductivity
p-value > 0.05	Pump Degradation

6.2.2   Ranking the Phenomena Following the Correlation Computation

After completing the correlation analyses for the LOFT study, we were able to numerically rank the phenomena from 1-5, with 1 representing the variable which was most strongly correlated with PCT and 5 being the variable which was least correlated with PCT. From an engineering perspective, we would rank the phenomena by absolute value of the change in PCT from the minimum value to the maximum value of the phenomena. To approximate that computation, we held the other phenomena at their respective nominal values. $\approx \Delta$t corresponds to the approximate change in temperature when we compare the PCT of the minimum value of the variable to the PCT of the maximum value of the variable, where all other variables are held constant at their respective nominal values. The following table presents the rankings:

36

Rank	Phenomena	$\approx \Delta$t (Rank by $\approx \Delta$t)
1	Fuel Clad Gap Width (G2)	200 (1)
2	Clad to Coolant Heat Transfer (G4)	80 (3)
3	Peaking Factor (G1)	50 (4)
4	Break Discharge Coefficient (G5)	90 (2)
5	Fuel Thermal Conductivity (G3)	45 (5)

The ranking by correlation coefficients almost matches the ranking we get by considering Δt- with the exception being that group 5 should be ranked number 2, and then the others would adjust accordingly. This seems to demonstrate that ranking using the correlation coefficients is fairly reasonable. Additionally, it may be worth noting that by the Apendix K ruling of the NRC, all of these correlation coefficients change in temperature would require that these phenomena be ranked 'high.'

7   Final Conclusions and Potential Future Work

Overall, in the AP600 studies, we found that Core Power was the dominating input parameter which most strongly affected our key output, but found that the significance of the variables after that were largely dictated by the break size. For the most part, we found that our statistical rankings were generally the same or less than the PIRT ranking, with the exception of VAR13 in one transient (the 6 inch break.) This makes sense as the PIRT was conservative, i.e. if the experts doing the ranking were unsure as to whether or not a particular phenomenon was medium or high, they tended to rank it high. With regards to the one odd case of the variable 13 ranking medium in the 6 inch break, this indicates that we should further examine this variable and phenomenon. It may be that changing this variable actually relates to another phenomena not covered in the PIRT, or that this particular variable is more complex than we originally thought. One of the limitations of our study is that we cannot be sure how accurately our variables represent the phenomena. We

were limited by what quantities it made sense to adjust, as well as the fact that there were cases where we were unable to easily select variables to vary to correspond to phenomenon. In any case, the study does demonstrate great potential for further studies, in particular in applications to other PIRT analyses.

In the LOFT studies, we found that fuel clad gap width was most strongly correlated with the PCT, and interestingly enough, found that the pump degradation seemed to have no relation to Peak Clad Temperature.

Through utilization of PIRTs and statistical methods, we believe that a more accurate uncertainty analysis can be performed.

Further studies may demonstrate that the utilization of statistical methods may improve upon the accuracy of PIRTs produced by a panel of experts. Other future work may utilize the concepts of sampling reduction techniques to vary a greater number of parameters which maintaining a relatively small run-time for studies. Additional improvements to the input file generator may include the addition of the ability for the user to specify a larger number of distributions for the values of various variables.

Aknowledgements

and guidance regarding phenomena.

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Appendices

A   Input Modification Program

```
1    program input_mod
2    !
3    !COGNIZANT:  Alexandra E. Gertman
4    !CREATED:    2/22/2012
5    !UPDATED:    5/02/2012
6    !————————————————————————————————————————————————
7    !PROGRAM DESCRIPTION:
8    !   This program was created to generate many input files with varying
9    !   parameters (i.e. phenomena or variables).
10   !
11   !   The program generates an executable (a.out) upon compilation.
12   !
13   !   The executable (a.out) is combined with a marked input file as
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14  !   well as a study specification file (spec file) to create the
15  !   new input files.
16  !
17  !   A spec file includes:
18  !              -if the spec_file should generate new spec_files OR
19  !               if it should generate input files
20  !              -the base name of each generated input file
21  !               (base name also serves to indicate the name of
22  !               the marked input file)
23  !              -the number of variables
24  !              -the  number of jobs the combinations will be split
25  !               into
26  !              -which set of combinations this particular spec_file
27  !               will generate
28  !              -the number of groups of variables
29  !               (there are some cases when variables MUST be changed
30  !                simultaneously- in those cases, those variables
31  !                will all be grouped together)
32  !              -the name of each variable
33  !              -variable information such as distribution which
34  !               allow the program to make necessary calculations
35  !               to calculate the values each variable in the
36  !               spec file should experience, as well as the group
37  !               number each variable belongs to.
38  !
39  !   The executable will produce a file containing the run information
40  !   (run_layout) which specifies the number of input files that will
41  !    be built in each of the 'input file generator' spec files.
42  !
43  !   If the spec file is a 'spec file generator' spec file, when
44  !   compiled with the executable, it will create 'input file
45  !   generator' spec files (the number of which is specified in the
46  !   'spec file generator' spec file.
47  !
48  !   If the spec file is an 'input file generator' spec file, when
49  !   compiled with the executable, it will create new input files
50  !   based upon the marked input file and the specifications in
51  !   the spec file itself. Once compiled using the executable, it
52  !   will create a comb file (which it writes to as it creates each
53  !   of the input files) that contains all of the 'run information'
54  !   for each of the input files being generated.
55  !
56  !
57  !PROGRAM OUTLINE:
58  !
59  !1. Initialize variables, obtain and bypass the name of the executable file,
60  !    and read the command line option.
61  !
62  !2. Open the files.
63  !    2.1 Open spec_file - a file that has info about the study.
64  !        2.1.1 Read spec_file and the following information:
65  !              2.1.1.a. Whether the spec file is an 'input file generator' OR
66  !                       a 'spec file generator.'
67  !              2.1.1.b. BASE Name for the input files
68  !              2.1.1.c. Number of variables, number of 'input file generator'
69  !                       spec files that will be used in the study (i.e. njobs), which
70  !                       particular 'input file generator' the spec file is (i.e.
71  !                       combSet), and the number of groups of variables in the study.
72  !              2.1.1.d. Name of each variable (as it is marked in the file- except
73  !                       for the '$'- that is added immediately after the data is
74  !                       read-in. i.e. 'VAR1' becomes '$VAR1'.)
75  !              2.1.1.e. Minimum and Maximum values of each variable
76  !              2.1.1.f. Standard Deviation of each variable
77  !              2.1.1.g. Number of data points within the range
78  !              2.1.1.h. Probability function name (uniform, nromal, lognormal, ....).
79  !                       NOTE: Currently only uniform is available.
80  !              2.1.1.i. Group number each variable belongs to.
81  !        2.1.2 Calculate the number of possible combinations, and create an array based on njobs
82  !              and nposscombs which specifies which runs will take place on each combSet.
83  !        2.1.3 Create the file run_layout. Write nposscombs on line 1, and then write the
84  !              number of combinations in each combSet onto line 2. The file is then closed.
85  !        2.1.4 Based on the first line of the spec_file, one of 3 things will occur:
86  !              (1) If the spec_file's first line says "generate" send to the subroutine
87  !                  spec_gen. spec_gen will generate njobs of spec_files which have "run"
88  !                  instead of "generate" and have different combSet numbers. i.e. only
89  !                  the first two lines of the newly generated spec_files will differ
90  !                  from the original spec_file. Once generation  is done, program will
91  !                  terminate.
92  !              (2) If first line doesn't say 'run' or 'generate', program will terminate.
93  !              (3) If the first line is "run", the program will execute normally. i.e.,
94  !                  Follow the remainder of the outline.
95  !    2.2 Name of marked_input_file is created.
96  !    2.3 Open marked_input_file
97  !
98  !3. Generate input files
99  !   3.1 Calculate the variable values for each interval with 'uniform' distribution.
100 !       3.1.1 Calculate the interval length and increment size
```

41

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101  !        3.1.2  Use the probability function, minimum, interval length,
102  !               and increment size to calculate all the values the variable
103  !               will have and save these in an array.
104  !    3.2 Input file generation through loops and subroutines.
105  !        3.2.1 Make columns an array of ones (of size ngroups.)
106  !        3.2.2 Open var_val_comb (i.e. comb file)
107  !    3.3 Input file name generation and input file creation through subroutines.
108  !        3.3.1 Generate a file names based on combination number or var value.
109  !              For example: 'edhtrk99' vs 'edhtrk_11_3_3 '.
110  !        3.3.2 Call the subroutine index_gen to generate all the files.
111  !               -As each file is generated, the run number (i.e. comb_number) and
112  !                the values for each variable in that particular run/input file will
113  !                be written to the comb file.
114  !4. Close all files (with the exception of file 8, fileName, which is closed in the
115  !   subroutine copy_file or the subroutine spec_gen).
116  !———————————————————————————————————————————————
117  !
118  !   Data Dictionary
119  !
120  !   baseFileName       = a character (of size 10) indicating the name of RELAP5-3D
121  !                        input file, will serve as beginning letters of all generated
122  !                        input files. Additionally, it will serve as the beginning of
123  !                        the name of the file var_val_comb.
124  !   charCombNum        = a character (of size 8) which is a character conversion of
125  !                        the combination number of the run so that each line in the
126  !                        combination file starts with the run number for the
127  !                        specific combination of variables. It is a local variable
128  !                        in the recursive subroutine index_gen. It is padded with 0's
129  !                        to ensure that each run is EXACTLY 8 digits.
130  !   charCombSet        = a character of size 3 which is the character conversion of
131  !                        combSet. It is used so that the spec_file can be appended with
132  !                        the number corresponding to the set of combinations the spec
133  !                        file needs to generate. It's a local variable used in the
134  !                        subroutine spec_gen. It's also used in the main program to
135  !                        make the comb file specific to the combSet.
136  !   char_i             = a character (of size 8) which is a character conversion of
137  !                        columns(1:nvar) or (a character conversion of the combination
138  !                        number of the run) so that newFile can be appended with each
139  !                        particular variable's corresponding index for that
140  !                        combination. It is a local variable used in the subroutine
141  !                        name_gen, and is padded with 0's to ensure it each name is
142  !                        baseFileName_XXXXXXXX, where XXXXXXXX is EXACTLY 8 digits.
143  !   charlen            = a local integer in subroutine var_finder which is used to store
144  !                        the character conversion of the length of a particular var(i).
145  !                        It is used to re-write line with the variable value substituted
146  !                        in place of '$VARX'.
147  !   charvalu           = a local variable (of size 12) in subroutine var_finder which is
148  !                        the character conversion of valu. It allows valu to be appended
149  !                        to the file name.
150  !   columns            = an array of integers (of size nvar- originally set to 55) which
151  !                        stores the indices of variables in any given combination.
152  !                        columns(j) corresponds to jth value of variable j.
153  !   comb_number        = an integer indicating the combination number a particular
154  !                        generated input file corresponds to.
155  !   combSet            = an integer of size 3 indicating which particular set of
156  !                        combinations the given spec_file will need to generate.
157  !   ex                 = logical flag indicating existance of spec_file and
158  !                        marked_input_file.
159  !   exfile             = a character of size 10 indicating the name of the executable
160  !                        file (usually a.out unless otherwise specified at run time for
161  !                        input_mod.f90. NOTE: if the executable is changed, the user is
162  !                        advised to make corresponding changes to the python script
163  !                        (run_xxxx.py) if tests will be made on the INL cluster.
164  !   flag               = a character of size 2. It is entered by user after executable file.
165  !                        If flag is not '-i' program will send error message to user and quit.
166  !   found              = a logical variable, used in the subroutine copy_file to test whether
167  !                        or not '$VAR' occured in the line (card) being copied in copy_file.
168  !   genRun             = character of size '10' which should be either 'run' or 'generate'.
169  !                        It is found on the first line of the spec_file and if genRun is
170  !                        'generate' the program will call the subroutine spec_gen. If it's
171  !                        'run' then the program will run normally.
172  !   groupNumb          = integer array of size 55 which stores the group number of each var.
173  !   i                  = integer used in various arguments (i.e. getarg, do loops, etc).
174  !   ierr               = integer used to detect an input error in reading the spec_file,
175  !                        marked_input_file, fileName (subroutine copy_file and subroutine
176  !                        spec_gen), and var_val_comb files.
177  !   increment_size_var = array of real numbers indicating the size of increment each
178  !                        particular variable value will increase by.
179  !   colindex           = integer indicating the index of a particular column. It is used in
180  !                        if statements in the subroutine indexgen
181  !   int_length_var     = array (of size 55) of real numbers indicating the size of the
182  !                        range of the values for each particular variable.
183  !   is                 = integer used to denote the number of command line arguments when
184  !                        the executable file is run (usually a.out is the executable)
185  !   j                  = integer used in various arguments (i.e. do loops, etc.)
186  !   job_inc            = real number which is used to determine the number of jobs that
187  !                        should be in each combSet. (i.e. job_inc = nposscombs/njobs).
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42

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188  !   line              = a character (of size 132) which is used in the subroutine copy_file
189  !                       to store each string of text from the marked_input_file and then is
190  !                       used to write the same string into fileName. It is then passed to
191  !                       the subroutine var_finder which searches line for the variable
192  !                       markers (ex: $VAR1). If it does contain the specific variable
193  !                       marker, var_finder will make the variable/value substitution, and
194  !                       pass line back to the subroutine copy_file. It is also used in the
195  !                       subroutine spec_gen to read in some of the spec_file lines.
196  !   marked_input_file = character of size 25 which corresponds to the name of the input
197  !                       file which has been "marked" or contains flagsindicating where the
198  !                       variables are that will be replaced with the values generated by
199  !                       this program. It is used as a template for generating new input
200  !                       files.
201  !   maxpts            = array (of size 55) of integers which indicate the maximum number
202  !                       of points in any variable's range.
203  !   mn                = array (of size 55)  of real numbers indicating the minimum value
204  !                       for each particular variable.
205  !   mx                = array (of size 55) of real numbers indicating the maximum value
206  !                       for each particular variable. Also used locally in subroutine
207  !                       spec_gen
208  !   nameGenType       = a character (of size 4) indicating whether the user would prefer
209  !                       to generate names based on the total number of combinations
210  !                       ('comb') or the number of values for each variable ('var').
211  !                       Ex: 'ed3htrk_99' vs 'ed3htrk_11_3_3'
212  !   newFile           = a character (of size 80) which corresponds to the name of the new
213  !                       file which is generated by the subroutine name_gen
214  !   ngroups           = an integer indicating the number of groups of variables within a
215  !                       given file. To be more explicit, there are cases in which entire
216  !                       groups of variables must be changed SIMULTANEOUSLY, and those
217  !                       variables will be 'grouped' together. e.g. if vars 1-4 must change
218  !                       simultaneously, var 5 changes independently, vars 6-12 change
219  !                       simultaneously and var 13 changes independently then there are
220  !                       4 groups.
221  !   nposscombs        = integer indicating the total number of combinations that exist for
222  !                       writing one value for each variable (i.e. this will indicate the
223  !                       number of input files which will need to be generated.)
224  !   npts              = array (of size 55) of integers indicating the number of values
225  !                       each variable will have.
226  !   nruns             = array (of size 55) of integers which indicate the number of runs
227  !                       which are in each combSet. (i.e. nruns(2) = the number of runs in
228  !                       the 2nd combSet. The number of generated files will be
229  !                       nruns(combSet) - nruns(combSet-1).)
230  !   nvar              = integer indicating the number of variables which will be replaced
231  !                       in the marked_input_file. Also used in subroutine spec_gen.
232  !   originalFile      = a character (of size 10) which is used by the subroutine name_gen
233  !                       to denote the file which will be copied.
234  !   prob              = array (of size 55) of characters (of size 8) which indicate the
235  !                       type of probability distribution that will be used to determine
236  !                       where the points in the interval for each variable will be.
237  !   run_layout        = the name of the file containing the run information (i.e the
238  !                       number of combinations and the number of files created for each
239  !                       of the combSets. It is a character of size 10.
240  !   runLayout         = an array of size 55, which holds information about the number of
241  !                       runs that are in each combSet. It is written to the file run_layout
242  !                       and then utilized by the python script.
243  !   sp                = a character of size 1 (" ") used locally in the subroutine var_finder
244  !                       to add an extra space in the line (card) after the value of the variable
245  !                       is inserted AND to add an extra space to the variable name. This prevents
246  !                       the program from replacing '$VAR11's values with '$VAR1's values, as well
247  !                       as preventing errors in value replacement- previously, errors occurred
248  !                       as '$VARX' would replace correctly, but '$VARXY' would add a 'Y' to the
249  !                       beginning of the value replacement.
250  !   spec_file         = character of size 20 which corresponds to the name of the file
251  !                       which contains information about each of the variables which are
252  !                       going to be replaced in the marked_input_file. This information
253  !                       includes baseFileName, combSet, genRun, mn, mx, npts, nruns, nvar,
254  !                       stdev, and var. If genRun = 'generate' spec_file is used as a
255  !                       template for the generated spec files and serves as a base for the
256  !                       naming scheme of the newly generated spec files.
257  !   stdev             = array (of size 55) of real numbers indicating the standard
258  !                       deviation of each variable.
259  !   val               = array of real numbers (of size (20,55)) which corresponds to
260  !                       val(i,j) = value i of variable j from spec_file formula.
261  !   valu              = an array of size nvar which holds the specific array of values
262  !                       for a generated combination of variables and values (i.e.
263  !                       valu(j) = val(columns(j),j)). It is created in the subroutine
264  !                       index_gen and then passed to the subroutine copy_file, and then to
265  !                       the subroutine var_finder so that these values are plugged in for
266  !                       the specific variable in a particular copyFile.
267  !   var               = array (of size 55) of characters (of size 8) denoting each
268  !                       variable name
269  !   var_val_comb      = character of size 20 indicating the name of the file created that
270  !                       contains all the nposscombs of values of the different variables.
271  !                       In the file, column 1 corresponds to the values of variable 1,
272  !                       column 2 corresponds to the values of variable 2, etc. Each row
273  !                       represents a different combination (i.e. nposscombs rows and nvar
274  !                       columns)
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43

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275  !   where                   = an integer corresponding to a local variable in subroutine
276  !                             var_finder which holds the value returned by the index function
277  !                             (either a '0' or a '1') which indicates if the variable flag
278  !                             (ex: $VAR1) is within a particular line.
279  !———————————————————————————————————————
280  !
281  !   files
282  !
283  !   file unit number  = file name
284  !
285  !   1                       = spec_file (opened and closed in input_mod, utilized in the
286  !                             subroutine spec_gen if genRun = 'generation'.)
287  !   2                       = marked_input_file (opened and closed in input_mod, read in
288  !                             the subroutine copy_file.)
289  !   3                       = var_val_comb file (opened and closed in input_mod, written
290  !                             in the recursive subroutine index_gen.)
291  !   8                       = fileName. This is the file which is a copy all of  information
292  !                             from the marked_input_file or the information for spec_file if
293  !                             genRun = 'generate'. (It is opened, written, and closed
294  !                             in the subroutine copy_file, or in the subroutine spec_gen.)
295  !   9                       = run_layout. This is the file which contains the information about
296  !                             the runs it allows the user to double check that the comb files
297  !                             generated contain the correct number of runs. The first line is
298  !                             nposscombs. The second line is the array runLayout, with each
299  !                             integer in the array being size 4. It was originally created to
300  !                             be used in the python script, but we ended up not using it in
301  !                             that capacity.
302  !———————————————————————————————————————
303  !
304  !   program/subroutine names and descriptions
305  !
306  !   name                    = description
307  !
308  !   copy_file           = subroutine which is called by index_gen. It is passed (and
309  !                             returns) fileName, var, nvar, and valu. It is used to generate
310  !                             a copy of a marked input deck. In order to substitute in correct
311  !                             variable values, it calls the subroutine var_finder.
312  !   index_gen           = recursive subroutine called by input_mod. It is passed (and
313  !                             returns) baseFileName, index, columns, maxcolumn, nvar,
314  !                             nposscombs, val, var, comb_number, and nameGenType. It
315  !                             recursively generates all of the possible combinations of
316  !                             variables and values. It calls the subroutines copy_file (which
317  !                             calls var_finder) and name_gen to generate all of the
318  !                             input decks for a particular "input generator" spec file.
319  !   input_mod           = main program. It opens (and saves information from) spec_file.
320  !                             It generates the points for a uniform distribution, and it
321  !                             calls the recursive subroutine index_gen to generate the
322  !                             files corresponding to the variable/value combinations unless
323  !                             the first line of the spec file is 'generate' in which case,
324  !                             the program will call spec_gen to generate all of the 'input
325  !                             generator' spec files.
326  !   name_gen            = subroutine called by index_gen. It is passed (and returns)
327  !                             originalFile, columns, nvar, newFile, comb_number, and
328  !                             nameGenType. It is used to generate a newFile name which
329  !                             indicates the particular variable value combination of the
330  !                             file being created/copied if nameGenType = 'var', otherwise
331  !                             nameGenType = 'comb' and the generated name  will correspond to
332  !                             which combination number the file corresponds to.
333  !   spec_gen             = subroutine which is passed (and returns) spec_file, genRun,
334  !                             baseFileName, nvar, and combSet. It is called by the main program
335  !                             if genRun = "generate". It will create njobs specfiles which have
336  !                             the first line changed to 'run' as opposed to 'generate', so that
337  !                             when these new spec files are run, they will call index_gen and
338  !                             are able to generate the new input files. Additionally, it will
339  !                             generate njobs of them, each of which will have a different
340  !                             combSet value. (e.g. if njobs = 9, then one file will have combSet=1,
341  !                             one file will have combSet=2, ..., one file will have combSet=9.)
342  !   var_finder          = subroutine which is passed (and returns) line, var, nvar and valu.
343  !                             It is called by copy_file, and uses the above information to find
344  !                             the VARIABLE MARKERS in the file and substitutes the desired values
345  !                             into the line and then passes the edited line back to copy_file.
346  !———————————————————————————————————————
347  !
348  !   INFORMATION FOR THE USER:
349  !   1. THE MARKED INPUT FILE AND SPEC FILE (VARIABLE NAMING):
350  !       Add a '$' to the beginning of EVERY variable name in your marked input file
351  !       (i.e. template input file). In the SPEC FILE, place the variable WITHOUT the
352  !       '$' (i.e. in MARKED INPUT '$VAR1' in SPEC FILE 'VAR1') as a '$' is added in
353  !       in the main program immediately following the read statement (see sec 2.2.1).
354  !   2. VARIABLE NAMES:
355  !       In the program, variable names are set to be of size 8. HOWEVER, due to the
356  !       addition of '$' to the beginning of the variable name (see #1 directly above)
357  !       and due to the SPACE added to the end of the variable name (see the subroutine
358  !       var_finder for a more detailed explanation) variable names MUST be no more
359  !       than 6 CHARACTERS LONG.
360  !   3. NUMBER OF VARIABLES OCCURING WITHIN A CARD:
361  !       Currently ONLY 7 instances of variables may appear in a given line (regardless
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44

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362  !       of which variables− it could be the same variable multiple times plus a few
363  !       others, or all one variable, or all different variables a single line, i.e.
364  !       card, may only have 7 substitutions). For more details, see the subroutine
365  !       var_finder.
366  !    4. CASE OF A VARIABLE WITH A SINGLE POINT (i.e. stays constant):
367  !       In the SPEC FILE, simply write the value the user desires to remain constant
368  !       for that variable in the place where the MIN (i.e. mn) should go.
369  !    5. MAX NUMBER OF RUNS:
370  !       Currently ONLY runs of up to 8 digits long are permitted. To change this, and
371  !       for additional information see NOTE in recursive subroutine index_gen.
372  !    6. MAXIMUM NUMBER OF VARIABLES SPECIFIED in SPEC FILE:
373  !       Currently a spec file can ONLY contain information for 55 variables. To
374  !       change this, the user will need to change the size of several arrays:
375  !       prob(XX), var(XX), columns(XX), groupNumb(XX), npts(XX), nptsGroup(XX),
376  !       nruns(XX), runLayout(XX), increment_size_var(XX), int_length_var(XX),
377  !       mn(XX), mx(XX), stdev(XX), val(20,XX), as well as in a write statement
378  !       [write (9, '(XXi4)')]. Additionally, changes should be made in the
379  !       recursive subroutine index gen: val(20,XX), and 62 format(a8,XXes12.4)
380  !       ALSO should more than 99 variables be in a given file, additional changes will
381  !       need to be made in   var_finder. See the subroutine for further details.
382  !−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−
383  !
384  !   Declarations
385  !
386        implicit none
387        character *10 baseFileName, exfile, genRun, run_layout
388        character *3 charCombSet
389        character *2 flag
390        character *25 marked_input_file
391        character *4 nameGenType
392        character *8  prob(55), var(55)
393        character *20 spec_file, var_val_comb
394        integer combSet, comb_number, i, ierr, is, j, k, maxpts, nposscombs, ngroups,  njobs, nvar
395        integer columns(55), groupNumb(55), npts(55), nptsGroup(55), nruns(55), runLayout(55)
396        logical ex
397        real increment_size_var(55), int_length_var(55), mn(55), mx(55), stdev(55), val(20,55)
398        real job_inc
399  !−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−−
400  !
401  !   Executable code
402  !
403  !   1.0 Initialize
404        comb_number = 0
405        genRun = 'hello'
406        i = 0
407        j = 0
408        maxpts = 1
409        nameGenType = 'type'
410        nposscombs = 1
411        var_val_comb = 's'
412  !
413  !   1.1 Obtain and bypass the name of the executable file
414        call getarg (i, exfile)
415        is = iargc()
416  !
417  !   1.2 Read the command option
418        i = 1
419        call getarg (i, flag)
420        if (flag(1:2) == "−i") then
421          i = 2
422          call getarg (i, spec_file)
423        else
424          write (*,*) "Error:_no_−i_was_specified"
425          stop "−1"
426        endif
427  !
428  !   2.0 Open the files
429  !
430  !   2.1 Open spec_file
431        inquire (file = spec_file, exist = ex)
432        if (.not. ex) then
433          write (*,*) "Error:_file_not_found,_", spec_file
434          go to 100
435        endif
436        open (unit = 1, file = spec_file, action = "read", status = "old", iostat = ierr)
437  !
438  !   2.1.1 Read the spec_file and save the relevant variable information. Then rename
439  !         each variable to include marker (i.e. '$').
440        read (1, "(a10)") genRun
441        read (1, "(a10,i3,i3,i3,i3)") baseFileName, nvar, njobs, combSet, ngroups
442        do i = 1, nvar
443          read (1, "(a8,_3e12.4,_i3,_a8,_i3)", end = 10) var(i), mn(i), mx(i), stdev(i), npts(i),&
444  prob(i), groupNumb(i)
445          var(i) = "$" // trim(var(i))
446        end do
447  10  continue
448        rewind 1
```

45

```fortran
449  !   2.1.2 Calculate the number of possible combinations, and create an array based on njobs
450  !         and nposscombs which specifies which runs will take place on each combSet.
451  !         For example: if there are 27 possible combinations, and njobs = 3, then
452  !         nruns( ) = [3  6  9], so we know combinations 1-3 will take place if combSet = 1,
453  !         combinations 4-6 will take place if combset = 2, and combinations 7-9 occur when
454  !         combSet = 3. Since the ceiling function is used, any number of njobs may be used
455  !         without concern for the case where  njobs does not evenly divide nposscombs. In
456  !         that case,  we will just have a different   number, i.e.  +/- 1, of runs generated
457  !         in one of the 'input deck generator' spec files.)
458  !
459      k = 1
460      nptsGroup(1) = npts(1)
461      do i = 1, nvar
462         if (groupNumb(i) /= groupNumb(k)) then
463            k = k + 1
464            nptsGroup(k) = npts(i)
465         endif
466      end do
467  !   uncomment the line below to write out the group number of each variable
468  !   write (*,"(20i4)") groupNumb
469  !
470      nposscombs = 1
471      do i =1, ngroups
472         nposscombs = nptsGroup(i)*nposscombs
473      end do
474  !
475      job_inc = (nposscombs)/(njobs)
476  !
477      do i = 1, njobs-1
478         nruns(i) = i*ceiling(job_inc)
479      end do
480      nruns(njobs) = nposscombs
481  !
482  !   2.1.3 Open the file "run_layout". It will be used by the python script.
483  !         For the file, we'll print out the number of possible combinations
484  !         (i.e. the total number of tests). Then we'll calculate exactly how
485  !         many runs are expected for each of the nodes (i.e. for each combSet),
486  !         and then write that onto the second line. (each will be of size 4).
487  !         Note: npossCombs will be of size 12. The file will then be closed.
488  !
489      run_layout = "run_layout"
490      open(unit = 9, file = run_layout, action = "write", status = "replace", iostat = ierr)
491      write(9, "(i12)") nposscombs
492      runLayout(1) = nruns(1)
493      do i = 2, njobs
494         runLayout(i) = nruns(i) - nruns(i-1)
495      end do
496      write(9, '(55i4)') runLayout(1:njobs)
497      close(unit = 9)
498  !
499  !   2.1.4 Based on genRun, program will follow one of three options.
500  !         (1) If spec_file is a spec_file with a genRun= "generation", send the spec_file
501  !             to the subroutine spec_gen which will generate njobs of spec_files. (first if)
502  !         (2) If spec_file's genRun is not equal to "run" program will terminate
503  !         (3) Otherwise, execute normally, utilizing the subroutine index_gen.
504  !
505      if (trim(genRun) == 'generate') then
506         call spec_gen(spec_file, genRun, baseFileName, nvar, njobs, combSet, ngroups)
507         go to 100
508      elseif (trim(genRun) /= 'run') then
509         go to 100
510      endif
511  !
512  !   2.2 Use the baseFilename as the marked_input_file
513  !
514      marked_input_file = trim(baseFileName) // '.i'
515  !
516  !   2.3 Open the marked_input_file
517      inquire (file = marked_input_file, exist = ex)
518      if (.not. ex) then
519         write (*,*) "Error: file not found, ", marked_input_file
520         go to 100
521      endif
522      open(unit =2, file = marked_input_file, action = "read", status = "old", iostat = ierr)
523  !
524  !   3. Generate input files.
525  !
526  !   3.1 Calculate the variable values for each interval with 'uniform' dist
527  !
528  !   3.1.1 Calculate the interval length and increment size
529  !
530      do i = 1, nvar
531         int_length_var(i) = mx(i) - mn(i)
532         if (npts(i) <= 1) then
533            increment_size_var(i) = 0.0
534         else
535            increment_size_var(i) = int_length_var(i)/(npts(i)-1)
```

```fortran
536        endif
537      end do
538 !
539 !   3.1.2  Calculate  each  value  within  the  interval  for  each  specific  variable.
540 !         Note:  val(rownumber = point in interval , column = variable ).
541      do i = 1, nvar
542        do j = 1, npts(i)
543          val(j, i) = mn(i) + (j-1)*(increment_size_var(i))
544        end do
545 !    uncomment the line below to write out all the values for each variable
546 !      write (*,*) "Values for variable ", trim(var(i)), ": ", val(1:npts(i),i)
547      end do
548 !
549      maxpts = 1
550      maxpts = maxval(nptsGroup)
551 !
552 !   3.2  Input  file  generation  through  loops  and  subroutines.
553 !
554 !   3.2.1  Make columns an array of size ngroups with all 1's (ones) inside
555      columns(1:ngroups) = 1
556 !
557 !   3.2.2  Open var_val_comb , and make the name specific to the combSet by
558 !          writing a character version of combSet and then appending that
559 !          to the trimmed version of baseFileName and the string "_comb".
560      write(charCombSet,'(i3)') combSet
561      charCombSet = trim(charCombSet)
562      var_val_comb = trim(baseFileName) // "_comb"// adjustl(charCombSet)
563      open(unit = 3, file = var_val_comb, action = "write", status = "replace", iostat = ierr)
564 !
565 !   3.3  Input  file  name  generation  and  file  creation  through  subroutines.
566 !
567 !   3.3.1  Generate  file  names  based  upon  the  number  of  combinations  of
568 !          variables and values or based on the possible values of each
569 !          variable. nameGenType has two values 'comb' and 'var'.
570 !          Ex: 'edhtrk_99' for 'comb' vs 'edhtrk_11_3_3' for 'var'.
571      nameGenType = 'comb'
572 !
573 !   3.3.2  We call the subroutine index_gen. It , in turn , will call the subroutines
574 !          name_gen and copyfile (copyfile will then call the subroutine var_finder).
575 !          index_gen will generate all of the possible combinations of input variables
576 !          and will create all of the input files for the specific 'input file generator'
577 !          spec file by using name_gen and copyfile/var_finder.
578 !
579      call index_gen(baseFileName, ngroups, columns, nptsGroup, nvar, nposscombs, val, var,&
580 comb_number, nameGenType, nruns, combSet, groupNumb)
581 !
582 !   4. Close the spec_file , marked_input_file , and var_val_comb file
583      close (unit = 1, status = "keep")
584      close (unit = 2, status = "keep")
585      close (unit = 3, status = "keep")
586 100 stop
587
588 contains
589
590 recursive subroutine index_gen (baseFileName, colindex, columns, maxcolumn, nvar, nposscombs, val,&
591 var, comb_number, nameGenType, nruns, combSet, groupNumb)
592 !
593 !   AUTHORS: Dr. George L. Mesina and Alexandra E. Gertman
594 !   CREATED: Mar 02, 2012
595 !   UPDATED: Apr 18, 2012
596 !
597 !   RECURSIVE SUBROUTINE DESCRIPTION:
598 !   Recursively generate an colindex (columns) which corresponds to the
599 !   matrix of variable values. ( i.e. val(columns(j), j) corresponds to
600 !   the column(j) value of variable j.) Then call the subroutines
601 !   name_gen and copy_file (copy_file will also call var_finder) to
602 !   generate the corresponding input file names and files.
603 !
604 !   CAUTION:
605 !   Note that combSet == 1 is handled differently than combSet > 1!
606 !   if changes must be made to the lines written to the combfile ,
607 !   user should ensure that changes are made to the case when
608 !   combSet == 1 AND combnumber > nruns(combSet-1).
609 !
610 !   NOTE:
611 !   comb_number (specifically the character version of comb_number,
612 !   charCombNum) is not currently able to handle comb_number > 8 digits.
613 !   if user wishes to change this , changes need to be made to several
614 !   places:
615 !        (i)  index_gen
616 !                       1. size of character charCombNum in declarations
617 !                          of local vars from '*8' to '*X'
618 !                       2. in write statement where comb_number is written to
619 !                          the charCombNum '(i8.8)' to '(iX.X)' for BOTH elseif
620 !                          cases.
621 !                       3. in format 62 and 87 change 'a8' to 'aX'
622 !        (ii) name_gen
```

47

```fortran
623  !                           1. size of char_i in declarations to '*X'
624  !                           2. in the write statement where comb_number is written to
625  !                              char_i, the format should be changed from '(i8.8)' to
626  !                              '(iX.X)'.
627  !
628  !   Declarations
629  !
630  !   Arguments
631      implicit none
632      character *10 baseFileName
633      character *4 nameGenType
634      character *80 newFile
635      character *8 var(*)
636      integer columns(*), groupNumb(nvar), maxcolumn(*), nruns(*)
637      integer combSet, comb_number, colindex, nvar, nposscombs
638      real val(20, 55)
639  !
640  !   Local Variables
641      integer i, j
642      real valu(nvar)
643      character *8 charCombNum
644  !
645  ! Initialize
646      newFile = baseFileName
647  !
648  !   Executable Code
649  !
650      if (colindex == 1) then
651        do i = 1, maxcolumn(1)
652          columns(1) = i
653          do j = 1, ngroups
654            where (groupNumb == j) valu = val(columns(j),:)
655          end do
656          comb_number = comb_number + 1
657  !       if (comb_number > 6) stop
658  !  Remove line above to generate more than 2 input files.
659          if (comb_number > nruns(combSet)) then
660            stop
661          elseif (combSet == 1) then
662            call name_gen(baseFileName,columns(1:nvar),nvar,newFile, comb_number,nameGenType)
663            call copy_file(newFile, var, nvar, valu)
664            write (charCombNum, '(i8.8)') comb_number
665            write (3,62) charCombNum, valu(1:nvar)
666            62 format (a8, 55es12.4)
667            ! write (3,621) charCombNum, (columns(j),j=1,ngroups)
668            ! uncomment line above (and below) to write the index of each group for each run
669            ! 621 format (a8, 55i3)
670          elseif (comb_number > nruns(combSet-1)) then
671            call name_gen(baseFileName,columns(1:nvar),nvar,newFile, comb_number,nameGenType)
672            call copy_file(newFile, var, nvar, valu)
673            write (charCombNum, '(i8.8)') comb_number
674            write (3,62) charCombNum, valu(1:nvar)
675            ! write (3,621) charCombNum, (columns(j),j=1,ngroups)
676            ! uncomment line above (as well as the format line) to write the index of each group
677            ! for each run
678          endif
679        end do
680      else
681        do i = 1, maxcolumn(colindex)
682          call index_gen (baseFileName, colindex-1, columns, maxcolumn, nvar, nposscombs, val,&
683    var,comb_number, nameGenType, nruns, combSet, groupNumb)
684          columns(colindex) = columns(colindex) + 1
685        end do
686        if (columns(colindex) > maxcolumn(colindex)) then
687          columns(colindex) = 1
688        endif
689      endif
690      if (comb_number > nposscombs) then
691        stop
692      end if
693  return
694  !
695  end subroutine index_gen
696  !_____
697  !
698  subroutine copy_file(fileName, var,nvar,valu)
699  !
700  !   CREATED: Mar 6, 2012
701  !   UPDATED: Apr 11, 2012
702  !
703  !   SUBROUTINE DESCRIPTION:
704  !   Make (i.e. open and write to) a copy of the marked-up input file
705  !   with the generated name. Then call var_finder to modify fileName
706  !   so it's variable values correspond to the file name. Also appends
707  !   the file name to include '.i'
708  !
709  !   Declarations
```

```fortran
710  !
711  !    Arguments
712  !    Arguments
713      implicit none
714      character *80 fileName
715      character *8 var(*)
716      integer nvar
717      real valu(*)
718  !
719  !    Local Variables
720      character *132 line
721      integer ierr
722      logical found
723  !
724  !    Executable Code
725  !
726      open (unit = 8, file = fileName, action = "readwrite_", position = "rewind",&
727  status = "replace", iostat = ierr)
728      do
729         read (2, "(a132)", end = 999) line
730         found = index (line, "$VAR") > 0
731         call var_finder(line,var,nvar,valu)
732         write (8, "(a)") trim(line)
733  !
734  !      UNCOMMENT the text below to print out the line that was altered by
735  !      the subroutine var_finder and written into the NEW input file.
736  !
737  !      if (found) then
738  !             write (*,*) "Copy File : line = ", line
739  !      end if
740  !
741      end do
742
743      999 continue
744
745      close (unit = 8)
746
747      rewind 2
748
749      return
750
751  end subroutine copy_file
752  !—————————————————————————————————————————————————
753  !
754  subroutine name_gen(originalFile,columns,nvar,newFile, comb_number, nameGenType)
755  !
756  !    CREATED: Mar  7, 2012
757  !    UPDATED: Mar 19, 2012
758  !
759  !    SUBROUTINE DESCRIPTION:
760  !    Creates name for input files based on base name AND variables if
761  !    nameGenType = 'var', otherwise nameGenType = 'comb' and the name generated will
762  !    be based on the base name and combination number the var/val corresponds to.
763  !
764  !    Declarations
765  !
766  !    Arguments
767      implicit none
768      character *4 nameGenType
769      character *80 newFile
770      character *10 originalFile
771      integer columns(1:nvar)
772      integer comb_number, nvar
773  !
774  ! Local Variables
775      character *8 char_i
776      integer j
777  !
778  ! Executable Code
779  !
780      newFile = originalFile
781
782      if (nameGenType == 'comb') then
783        write(char_i, '(i8.8)')comb_number
784        newFile = trim(newFile) // "_" //trim(adjustl(char_i))
785      else
786        do j = 1, nvar
787          write(char_i, '(i2)') columns(j)
788          newFile = trim(newFile) // "_" // trim(adjustl(char_i))
789        end do
790      endif
791
792      newFile = trim(newFile) // '.i'
793
794      return
795
796  end subroutine name_gen
```

49

```fortran
797  !————————————————————————————————————————————
798  !
799  subroutine var_finder(line,var,nvar, valu)
800  !
801  !   CREATED: March 07, 2012
802  !   UPDATED: April 12, 2012
803  !
804  !   SUBROUTINE DESCRIPTION:
805  !   Find the lines in the input file which contain a variable MARKER
806  !   (i.e. '$VAR1') and then replace the MARKER with the desired value.
807  !
808  !   NOTE:
809  !   The variable name can have a double digit number, so special care
810  !   must be taken when forming the new line to prevent part of the
811  !   name from appearing in the new line. To handle this case, an
812  !   additional SPACE has been added to the END of the value replacing
813  !   the marked variable in the line. THIS could potentially cause errors
814  !   in input processing as it may cause there to be too many characters
815  !   on a card in the new input file.
816  !
817  !   LET THE USER BEWARE:
818  !   Currently, this subroutine is set to account for up to 7 occurences
819  !   of a variable within a single card (line) in the input deck.
820  !   IF more occurences exist in the user's modified deck, CHANGE the
821  !   outermost do-loop from 1 to 7  TO 1 to X (greatest number of
822  !   instances of variables occuring on a single card (line) in the marked
823  !   input deck.
824  !
825  !   ADDITIONAL WARNING:
826  !   ALL VARIABLES ($XXXXXX, where XXXXX is input by the user) are PADDED
827  !   with a SPACE (i.e. from '$XXXXX' to '$XXXXX ' within this subroutine)
828  !   so as to ENSURE that the program will not read in variables such as
829  !   '$VAR1' and '$VAR11' (assuming the user puts them in sequentially in
830  !   the spec file) and then replace all '$VAR11's values with '$VAR1's
831  !   values. The user should also be aware that we insert an extra space
832  !   in the line immediately following the value insertion. If the user
833  !   should have more than 99 variables, it is recommended that an extra
834  !   space be inserted for each additional digit of nvar (e.g. for 2000,
835  !   add two extra spaces, for 999 add one extra space.)
836  !
837  !   Declarations
838  !
839  !   Arguments
840      implicit none
841      character *132 line
842      character *8 var(*)
843      integer nvar
844      real valu(*)
845  !
846  !   Local Variables
847      integer charlen, i, j, loc
848      character *12 charvalu
849      character *1 sp
850  !
851  !   Executable Code
852  !
853      sp = "␣"
854      do j = 1, 7
855         do i = 1, nvar
856            loc = index (line, trim(var(i)) // sp)
857            if (loc .ne. 0) then
858               charlen = len_trim(var(i))
859               write (charvalu,"(es12.4)") valu(i)
860  !   UNCOMMENT the text below to check which variable and value is being
861  !   substituted into a particular line. NOTE that it will print out EACH
862  !   occurence of the variable being replaced.
863  !           write (*,*) "Var Finder : var(i) = ", var(i), i
864  !           write (*,*) "Var Finder : line before = ", line
865  !
866               line = line(1:loc-1) // charvalu // sp // line(charlen+loc+1:)
867  !
868  !           write (*,*) "Var Finder : line after = ", line
869  !
870            endif
871         end do
872      end do
873
874      return
875
876  end subroutine var_finder
877  !————————————————————————————————————————————
878  !
879  subroutine spec_gen(spec_file, genRun, baseFileName, nvar, njobs, combSet, ngroups)
880  !
881  !   CREATED: Mar 15, 2012
882  !   UPDATED: Apr 18, 2012
883  !
```

```fortran
884  !   SUBROUTINE DESCRIPTION:
885  !   Create njobs specfiles which have the first line changed to 'run'
886  !   as opposed to 'generate', so that when these new spec files are run,
887  !   they will call index_gen and actually generate the new input files.
888  !
889  !   Declarations
890  !
891  !   Arguments
892     implicit none
893     character *10 baseFileName, genRun
894     character *20 spec_file
895     integer combSet, ngroups, njobs, nvar
896  !
897  !   Local Variables
898     character *3 charCombSet
899     character *20 fileName
900     character *132 line
901     integer i, ierr, j
902  !
903  !   Executable Code
904  !
905     do i = 1, njobs
906
907        combSet = i
908        write(charCombSet,'(i3)') combSet
909
910        fileName = trim(spec_file) // '_' // adjustl(charCombSet)
911        fileName = trim(fileName)
912        open (unit = 8, file = fileName, action = "readwrite_", position = "rewind",&
913  status = "replace", iostat = ierr)
914  !
915  !   read in the first two lines of spec_file. At this point, we won't be
916  !   doing anything with them, but after we read them in, we'll be all set
917  !   to read in the rest of the lines (and print them out) in a loop.
918  !
919        read (1, "(a132)", end = 999) line
920        read (1, "(a132)", end = 999) line
921  !
922  !   write the first two lines of the new spec_file- replacing "generate" with
923  !   "run" and changing the combSet number appropriately.
924  !
925        write (8, "(a3)") "run"
926        write(8, 23) baseFileName, nvar, njobs, combSet, ngroups
927        23 format(a10, i3, i3, i3, i3, i3)
928        999 continue
929  !
930  !   now we read in the rest of the lines from file 1 and write with no
931  !   modifications onto the spec_file we're generating.
932  !
933        do j = 1, nvar
934          read (1, "(a132)", end = 99) line
935          write (8, "(a)") trim(line)
936        end do
937        99 continue
938
939        rewind 8
940        close (unit = 8)
941        rewind 1
942     end do
943     return
944  end subroutine spec_gen
945  !————————————————————————————————————————————
946  !
947  end program input_mod
```

B   Template Spec File

```
1  typeOfSpecFile

2  baseFileName #vars #nodesInStudy currentNode #groups

3  varX                  min    max    stdDev   #pts       distribution group#

4  .                                                    .

5  .                                                    .
```

```
6   .                                              .
7   .                                              .
8   varY                    min     max    stdDev    #pts       distribution  group#
```

C   Example of a Generator Spec File

```
1   generate
2   apsbs      8   9   6   8
3   VAR1    0.9              1.1           0.1              3   uniform  1
4   VAR2    0.000135         0.000165      0.000015         3   uniform  2
5   VAR3    10.63287         12.99573      1.18143          3   uniform  3
6   VAR4    0.036252         0.044308      0.004028         3   uniform  4
7   VAR5    0.14688          0.17952       0.01632          3   uniform  5
8   VAR6    0.078534         0.095986      0.008726         3   uniform  6
9   VAR7    0.000135         0.000165      0.000015         3   uniform  7
10  VAR8    .504811          0.616991      0.05609          3   uniform  8
```

D   Example of a NodeSpec File

```
1   run
2   apsbs      8   9   9   8
3   VAR1    0.9              1.1           0.0471404520     3   uniform  1
4   VAR2    0.00135          0.00165       0.0000707106     3   uniform  2
5   VAR3    8.95959          10.95061      0.4692879144     3   uniform  3
6   VAR4    0.043749         0.053471      0.0022914973     3   uniform  4
7   VAR5    0.193752         0.236808      0.0101483965     3   uniform  5
8   VAR6    0.04419          0.05401       0.0023145962     3   uniform  6
9   VAR7    0.000135         0.000165      0.0000070710     3   uniform  7
10  VAR8    .19493874        0.23825846    0.0102105559     3   uniform  8
```

E Python Script for Running Studies on INL's Supercomputer, Quark

```python
#!/apps/local/python/activestate/2.7.1.4/bin/python
#
#   Purpose: Run many input decks from many directories with RELAP5-3D
#   Note:     Pure Python script, no use of Linux scripts or commands.
#             To adjust this run_file for your particular test, go to
#             main program, section 1.0 and adjust the file names (and
#             keyOutputString) accordingly. The user is also encouraged
#             to adjust the walltime request to better fit the user's
#             study.
#   Authors: Dr. George L Mesina, Alexandra E. Gertman
#            J. Shelley
#   Created: Mar 16, 2012
#   Updated: May 02, 2012
#
#   Pro Batch Scheduler (PBS) commands
#PBS -N relap5
#PBS -l select=1:ncpus=12:mpiprocs=12:mem=23gb
#PBS -l place=excl
#PBS -l walltime=10:00:00
#PBS -V
#PBS -j oe
#PBS -q general
#
################################
#
#   1.0 Imports
import glob, os
from tempfile import mkdtemp
import shutil, subprocess, sys
from string import join
import time
try:
    import forkmap as fm
    FORKMAPavail = "yes"
except Exception, e:
    FORKMAPavail = "no"
################################

################################
def CreateDirs(curPath,outPath,filePre,tmpPath):
#   Make the directories where each node's (or combSet's)
#   cases will be run
#
    tmp_dir = mkdtemp(prefix=filePre, dir=tmpPath)
    return tmp_dir
################################

################################
def GetInputFiles(inputPre):
#
#   Grab all of files (each of which is named inputPre) from our current path.
#   Then return all of those files.
#   Note: inputPre = specFilePre + '*' for specFiles AND
#         inputPre = inputFilePre%"*"  for inputFiles
#
    inputs = glob.glob(inputPre)
    return inputs
################################

################################
def PrepRunGetClean(index, currentPath, relap_exe, tmpPath):
#
#   Runs each input file passed to it (using relap executable rund).
#   Currently, only 12 input files are run at a time (since we're running
#   our tests on quark.) If a different number should be run through each
#   time, appropriate changes should be made in the parallel section, as
#   as in the beginning lines of this program (the PBS -l  select line).
#
    cmd = "%s_%s"%(relap_exe,index)
    output = subprocess.Popen(cmd,shell=True,stdout=subprocess.PIPE).communicate()[0]
    print >> sys.stderr, 'cmd: ', cmd

    return
################################

################################
if __name__ == '__main__':
#   DESCRIPTION: Create working directory in temporary-space with subdirs
#                one per cluster node. Run input_mod_gen.f90 to create 1
#                spec-file for each subdirectory by dividing the total no.
#                of combinations equally among the cluster-nodes. Copy the
```

```
 82  #                    license and template input files , RELAP5-3D, and tpfh2o
 83  #                    to each subdirectory. Use input_mod_gen.f90 to generate
 84  #                    all input files for the node from template input file.
 85  #                        Find and store key output parameter value from each
 86  #                    RELAP5-3D output file along with the sequence number of
 87  #                    the file.
 88  #                        When all runs are finished , SAS will be used to
 89  #                    analyze the statistics.
 90  #
 91  #   COGNIZANT:    Alexandra E. Gertman, Dr George Mesina , Jon Shelley
 92  #   CREATED: Mar 16, 2012
 93  #   UPDATED: Mar 27, 2012
 94  #
 95  #   PROGRAM OUTLINE:
 96  #   1.0   Initialize and set-up directories
 97  #   1.1 Construct & Populate subdirectories
 98  #       Construct subdirectory structure explained above
 99  #       1.1.1 Change the current working directory to currentPath
100  #       1.1.2 Collect all of the spec files we'll use in this study.
101  #       1.1.3 If the directory (tmpPath) does not yet exist , create it.
102  #             Then create the directory which will hold all of the runs
103  #             for each combSet (i.e. for each node).
104  #   1.2 Obtain list of computer nodes
105  #   1.3 Input file generation
106  #       1.3.1 Switch the current working directory to tmp_run_dir
107  #             (i.e. the temporary directory)
108  #       1.3.2 In each temporary directory , create a link to the needed files:
109  #             the RELAP5-3D executable (rund), relap5.x, its license and property
110  #             files , and the appropriate specfile.
111  #       1.3.4 Collect all of the input files.
112  #   2.0 Output file generation through parallelization
113  #   2.1 Run Parallel: All of the input files that were
114  #       generated will be run with the relap executable.
115  #       2.1.1 Grab 12 of the input files at a time, passing them
116  #             to the function PrepRunGetClean where the output
117  #             for those 12 input files will be created.
118  # 3.0 Results
119  # 3.1 Collect the newly generated output files
120  #       3.1.1 Create a results dictionary where we'll store
121  #             the run number and the corresponding desired
122  #             output parameter.
123  #       3.1.2 Loop through output files to find the key output
124  #             parameter, and then put that value into the results
125  #             dictionary along with the corresponding run number
126  # 3.2 Find the file with the variable information for each
127  #       run, copy that information and put into a new file ,
128  #       appending the run information with the desired output
129  #       from the results dictionary. Then save the results file
130  #       to the current directory.
131  #       3.2.1 Open and read the comb file for this particular combSet/node
132  #       3.2.2 Create the list outline.
133  #             3.2.2.1 Loop through each line of combLine
134  #                     3.2.2.1.1 Split each line in each of the combFiles
135  #                     3.2.2.1.2 Append each line with it's corresponding result
136  #                     3.2.2.1.3 Place modified cline into the list outline
137  #       3.2.3 Save all of outline to res_text.
138  #       3.2.4 Open combFile.res , write all of res_text to it , then close the file.
139  #       3.2.5 Copy the file to the folder 'results' in the home directory
140  # 4.0 Remove temporary directory and exit program
141  #
142  # DATA DICTIONARY:
143  #   array_idx        = array of cluster nodes. Should correspond to the number of
144  #                      jobs specified in spec file. (3rd word on line 2 of the
145  #                      spec file.)
146  #   cline            = variable denoting each specific line in combLine. It is
147  #                      stripped and split , appended, and then put back together.
148  #   cmd              = variable which denotes arguments we'll be passing to the
149  #                      command line.
150  #   combFile         = name of the comb file for the particular combSet/node.
151  #                      It is combFilePre with arry_idx.
152  #   combFilePre      = base name for each comb file.
153  #                      For ex: 'apsbs2_comb'. No additional string w/in a string
154  #                      is specified.
155  #   combLine         = where each line of the combFile is stored (each line is a
156  #                      string.)
157  #   combn            = the run number of cline
158  #   currentPath      = PBS working directory.
159  #   data             = where the information for an output file is stored.
160  #   inputFilePre     = base name used in all of the input files.
161  #                      For example: 'apsbs_%s.i', where the %s indicates that we
162  #                      will specify a what string will get placed in between the
163  #                      underscore and the ".i"
164  #   index            = variable used to denote 12 different strings (each of which
165  #                      corresponds to a specific input file.) It is used in the
166  #                      parallel section , and passed to PrepRunGetClean so that each
167  #                      of the 12 input files will be run with rund.
168  #   inputFiles       = all of the generated input files (i.e. spec files which contain
```

```
169  #                           'run' as their first word on line 1) we'll be using in this
170  #                           study. To get all of these files, we call the function
171  #                           GetInputFiles, and pass it the string specFilePre + '*'.
172  #   fixd           = line in data which contains keyOutputString
173  #   keyOutputParam = the number in fixd which corresponds to the key output parameter
174  #                           we are grabbing from the output files.
175  #   keyOutputString = string which occurs right before the key output parameter
176  #                           value in the '.p' relap file.
177  #   markedInputFile = name of the marked input file input_mod_gen.f90 uses as a
178  #                           template for generating all of the input files.
179  #   output         = the results generated from running each of the input files with
180  #                           the relap executable (rund).
181  #   ouputFilePre   = base name used in all of the output files. It functions in
182  #                           the same way as the inputFilePre, except it's a '.p' file.
183  #   outFile        = each individual output file (from outputFiles)
184  #   outputFiles    = the generated output files are all stored here. They are
185  #                           outputFilePre%'*'.
186  #   outline        = list which stores each line of combLine (and appends each of
187  #                           the lines with the corresponding result from res_dict.)
188  #   outputPath     = location of output files
189  #   relap_exe      = name of the relap executable (i.e. how we'll run relap for
190  #                           each particular input file.)
191  #   res_dict       = results dictionary. Items in the results dictionary are stored
192  #                           as run number and then corresponding key output parameter
193  #                           generated for that particular run.
194  #                           For ex: ['00000044':'69.5519', '00000045':'69.5519', ... ]
195  #   resFile        = where the results file is opened, written to (res_text is
196  #                           written into the file), and closed.
197  #   resultsFile    = name of the results file (combFile + '.res')
198  #   res_text       = file where the list outline is written to.
199  #   runtime        = a call (in parallel section) to the function controller,
200  #                           passing in all of the input files (12 of them at a time).
201  #   specFilePre    = base name of the spec file (NOTE: this is not the spec file
202  #                           generator— rather it is the generated copies which contain
203  #                           'run' as the first word on line 1 of the spec file.)
204  #                           Unlike the input/output pre it doesn't include a string
205  #                           within a string.
206  #   specFiles      = all of the generated spec files (i.e. spec files which contain
207  #                           'run' as their first word on line 1) we'll be using in this
208  #                           study. To get all of these files, we call the function
209  #                           GetInputFiles, and pass it the string specFilePre + '*'.
210  #   start2         = floating point representation of time (used to denote when
211  #                           each set of 12 input files is run with RELAP.) It is used in
212  #                           the parallel section, in the function controller.
213  #   tmpPath        = location on temporary disk for the RELAP5-3D code and input
214  #   tmp_run_dir    = temporary directory where each node's (or combSet's) particular
215  #                           case will be run. It calls the function CreateDirs() to create
216  #                           each particular directory by passing currentPath, outputPath,
217  #                           as well as the specFilePre+str(arry_idx)+'-', and tmpPath)
218  #
219  ###############################
220  #
221  #   1.0   Initialize and set-up directories
222      arry_idx = int(os.environ['PBS_ARRAY_INDEX'])
223      currentPath = os.environ['PBS_O_WORKDIR']
224      tmpPath = "/tmp" + os.sep + "r5stats" + os.sep
225      outputPath = currentPath + os.sep + "Output" + os.sep
226      inputFilePre = "loftTS_%s.i"
227      outputFilePre = "loftTS_%s.p"
228      keyOutputString = "pct_____stdfnctn"
229      specFilePre = "loftTS_gen_"
230      markedInputFile = "loftTS.i"
231      relap_exe = "/home/gertae/hpc-runs/rund"
232      combFilePre = "loftTS_comb"
233  #
234      print >> sys.stderr, 'arry_idx:_',arry_idx
235      print >> sys.stderr, 'currentPath:_',currentPath
236      print >> sys.stderr, 'tmpPath:_',tmpPath
237      print >> sys.stderr, 'outputPath:_',outputPath
238  #
239  #
240  #   1.1 Construct & Populate subdirectories
241  #       Construct subdirectory structure explained above
242  #
243  #       1.1.1 Change the current working directory to currentPath
244      os.chdir(currentPath)
245      print "CWD:_",os.getcwd()
246      print "ls:_",os.listdir(os.getcwd())
247  #
248  #       1.1.2 Collect all of the spec files we'll use in this study.
249      specFiles = GetInputFiles(specFilePre+'*')
250      print "Spec_Files:_",specFiles
251  #
252  #       1.1.3 If the directory (tmpPath) does not yet exist, create it.
253  #             Then create the directory which will hold all of the runs
254  #             for each combSet (i.e. for each node).
255      if os.path.isdir(tmpPath) == False:
```

```
256            os.mkdir(tmpPath)
257        tmp_run_dir = CreateDirs(currentPath, outputPath, specFilePre+str(arry_idx)+'-',tmpPath)
258    #
259    #    1.2 Obtain list of computer nodes
260    #        Each node has a number of cores
261        nodes = open(os.environ['PBS_NODEFILE'],'r').readlines()
262        numNodes = len(nodes)
263        print "Number of threads: ",numNodes
264    #
265    #    1.3 Input file generation
266    #
267    #        1.3.1 Switch the current working directory to tmp_run_dir
268    #            (i.e. the temporary directory)
269        os.chdir(tmp_run_dir)
270    #        1.3.2 In each temporary directory, create a link to the needed files:
271    #            the RELAP5-3D executable (rund), relap5.x, its license and property
272    #            files, and the appropriate specfile.
273        for lnfile in ['rund','relap5.x','tpfh2o','rellic.bin', specFilePre+'%d'%arry_idx,
274                        markedInputFile]:
275            cmd = 'ln -s %s/%s'%(currentPath,lnfile)
276            print "cmd: %s"%cmd
277            output = subprocess.Popen(cmd,shell=True,stdout=subprocess.PIPE).communicate()[0]
278    #        1.3.3 In each temporary directory, create the command to
279    #            run the executable from input_mod_gen.f90 (a.out),
280    #            passing it '-i' (necessary for executable to work),
281    #            and specFilePre arry_idx.
282        cmd = currentPath+os.sep+'a.out -i %s%d'%(specFilePre,arry_idx)
283        print "cmd: %s"%cmd
284        output = subprocess.Popen(cmd,stdout=subprocess.PIPE,shell=True).communicate()[0]
285    #        1.3.4 Collect all of the input files.
286        inputFiles=GetInputFiles(inputFilePre%"*")
287        #inputFiles = inputFiles[:12] #Uncomment for smaller test
288        print inputFiles
289    #
290    #    2.0  Output file generation through parallelization
291    #
292    #
293    #    2.1  Run Parallel: This is where all of the input files that
294    #        were generated will be run with the relap executable rund.
295    #
296        ###################################
297        ## Parallel section
298        ###################################
299    #        2.1.1 Grab 12 of the input files at a time, passing them
300    #            to the function PrepRunGetClean where the output
301    #            for those 12 input files will be created.
302        @fm.parallelizable(12)
303        def controller(index):
304            print >> sys.stderr, 'index=',index
305            start2 = time.time()
306
307            PrepRunGetClean(index, currentPath, relap_exe, tmp_run_dir)
308
309            return time.time() - start2
310        runtime = fm.map(controller,[x for x in inputFiles])
311        ###################################
312        ## End Parallel section
313        ###################################
314        #
315    #
316    # 3.0 Results
317    #
318    # 3.1 Collect the newly generated output files
319        outputFiles = glob.glob(outputFilePre%'*')
320        print "Output Files: ",outputFiles
321    #        3.1.1 Create a results dictionary where we'll store
322    #            the run number and the corresponding desired
323    #            output parameter.
324        res_dict = dict()
325    #
326    #        3.1.2 Loop through output files to find the key output
327    #            parameter, and then put that value into the results
328    #            dictionary along with the corresponding run number
329        for outFile in outputFiles:
330            data=open(outFile).read()
331            fidx = data.rfind(keyOutputString)
332            keyOutputParam = (data[fidx:fidx+80]).split()[2]
333            #print "%s Coremin: %s"%(outFile,pct)
334            res_dict[outFile.split('-')[1].split('.')[0]]= keyOutputParam
335        print "Results Dictionary:\n",res_dict
336    #
337    # 3.2 Find the file with the variable information for each
338    #     run, copy that information and put into a new file,
339    #     appending the run information with the desired output
340    #     from the results dictionary. Then save the results file
341    #     to the current directory.
342    #
```

56

```python
343  #       3.2.1 Open and read the comb file for this particular combSet/node
344      print "Have_not_yet_found_Comb_File"
345      combFile=combFilePre+str(arry_idx)
346      print "Found_Comb_File"
347      combLine=open(combFile).readlines()
348  #
349  #       3.2.2 Create the list outline.
350      outline = list()
351  #
352  #             3.2.2.1 Loop through each line of combLine
353      for cline in combLine:
354  #
355  #                   3.2.2.1.1 Split each line in each of the combFiles
356          cline = cline.strip()
357          cline = cline.split()
358  #
359  #                   3.2.2.1.2 Append each line with it's corresponding result
360          try:
361              combn = cline[0]
362              cline.append(res_dict[combn])
363          except:
364              cline.append('noResults')
365  #
366  #                   3.2.2.1.3 Place modified cline [joined w/commas and w/ a
367  #                          '\n' at the end of the line to indicate a new
368  #                            line for each result] into the list outline
369          outline.append(",".join(cline) + "\n")
370  #
371  #    3.2.3 Save all of outline to res_text.
372      res_text = join(outline,'_')
373  #
374  #    3.2.4 Open combFile.res, write all of res_text to it, then close the file.
375      resultsFile=combFile+'.res'
376      print "Results_File(s):_", resultsFile
377      resFile = open(resultsFile,'w')
378      resFile.write(res_text)
379      resFile.close()
380  #
381  #    3.2.5 Copy the file to the folder 'results' in the home directory
382      shutil.copy(resultsFile,currentPath)
383  #
384  #    4.0  Remove temporary directory and exit program
385      try:
386          print "Remember_to_clean_up_after_the_run"
387          shutil.rmtree(tmpPath)
388      except Exception, e:
389          print >> sys.stderr, e
390          print >> sys.stderr, "Error_occurred_while_removing_temporary_directories"
391      #
392      print >> sys.stderr, 'Node_%i_runtimes_(sec):\n__Max_%f,\n__Min_%f,\n__Avg_%f,\n_Tot_%f_'%\
393          (arry_idx,max(runtime),min(runtime),sum(runtime)/len(runtime),sum(runtime))
394      print >> sys.stderr, "For_",len(runtime),"_runs"
395      RunTime = time.time() - Runstart2
396      print >> sys.stderr, "Total_run_time_=",RunTime
```

F   SAS Reports

F.1   AP600 2 inch Break, Top 4 Variables

Correlation Analysis

The CORR Procedure

1 With Variables:	coremin			
4 Variables:	VAR1	VAR8	VAR12	VAR13

SSCP Matrix				
	VAR1	**VAR8**	**VAR12**	**VAR13**
coremin	6607.808270	3294.217900	6618.107340	1.662016

CSSCP Matrix				
	VAR1	**VAR8**	**VAR12**	**VAR13**
coremin	-5.60623000	-12.48935000	4.69284000	-0.00787117

Covariance Matrix, DF = 80				
	VAR1	**VAR8**	**VAR12**	**VAR13**
coremin	-.0700778750	-.1561168750	0.0586605000	-.0000983896

Simple Statistics						
Variable	**N**	**Mean**	**Std Dev**	**Median**	**Minimum**	**Maximum**
coremin	81	81.64709	1.88027	81.67210	78.39860	84.71310
VAR1	81	1.00000	0.04108	1.00000	0.95000	1.05000
VAR8	81	0.50000	0.41079	0.50000	0	1.00000
VAR12	81	1.00000	0.24648	1.00000	0.70000	1.30000
VAR13	81	0.0002525	0.0002033	0.0002525	5E-6	0.0005000

Pearson Correlation Coefficients, N = 81 Prob > |r| under H0: Rho=0				
	VAR1	**VAR8**	**VAR12**	**VAR13**
	-0.90727	-0.20212	0.12658	-0.25734
coremin	<.0001	0.0704	0.2602	0.0204

Spearman Correlation Coefficients, N = 81 Prob > |r| under H0: Rho=0				
	VAR1	**VAR8**	**VAR12**	**VAR13**
	-0.90408	-0.21729	0.13451	-0.25932
coremin	<.0001	0.0513	0.2312	0.0194

Kendall Tau b Correlation Coefficients, N = 81 Prob > |tau| under H0: Tau=0				
	VAR1	**VAR8**	**VAR12**	**VAR13**
	-0.77650	-0.16867	0.10406	-0.20474
coremin	<.0001	0.0516	0.2298	0.0182

Hoeffding Dependence Coefficients, N = 81 Prob > D under H0: D=0				
	VAR1	**VAR8**	**VAR12**	**VAR13**
	0.31322	0.00025	-0.00573	0.00603
coremin	<.0001	0.3472	0.9429	0.1216

F.2 AP600: 4 inch Break, Top 5 Variables

Correlation Analysis

The CORR Procedure

1 With Variables:	coremin			
5 Variables:	VAR1 VAR8 VAR11 VAR12 VAR13			

SSCP Matrix					
	VAR1	VAR8	VAR11	VAR12	VAR13
coremin	16908.89162	8454.59730	16913.76764	16914.85865	4.26840

CSSCP Matrix					
	VAR1	VAR8	VAR11	VAR12	VAR13
coremin	-5.867280000	-2.782150000	-0.991260000	0.099750000	-0.002573307

Covariance Matrix, DF = 242					
	VAR1	VAR8	VAR11	VAR12	VAR13
coremin	-.0242449587	-.0114964876	-.0040961157	0.0004121901	-.0000106335

Simple Statistics						
Variable	N	Mean	Std Dev	Median	Minimum	Maximum
coremin	243	69.60806	0.76876	69.57290	68.11380	71.52660
VAR1	243	1.00000	0.04091	1.00000	0.95000	1.05000
VAR8	243	0.50000	0.40909	0.50000	0	1.00000
VAR11	243	1.00000	0.24545	1.00000	0.70000	1.30000
VAR12	243	1.00000	0.24545	1.00000	0.70000	1.30000
VAR13	243	0.0002525	0.0002025	0.0002525	5E-6	0.0005000

Pearson Correlation Coefficients, N = 243 Prob > |r| under H0: Rho=0					
	VAR1	VAR8	VAR11	VAR12	VAR13
	-0.77092	-0.03656	-0.02171	0.00218	-0.06831
coremin	<.0001	0.5706	0.7364	0.9730	0.2889

Spearman Correlation Coefficients, N = 243 Prob > |r| under H0: Rho=0					
	VAR1	VAR8	VAR11	VAR12	VAR13
	-0.76563	-0.03280	-0.01617	-0.00007	-0.05008
coremin	<.0001	0.6109	0.8020	0.9991	0.4371

Kendall Tau b Correlation Coefficients, N = 243 Prob > |tau| under H0: Tau=0					
	VAR1	VAR8	VAR11	VAR12	VAR13
	-0.61577	-0.02295	-0.01218	0.00229	-0.03845
coremin	<.0001	0.6436	0.8060	0.9632	0.4382

Hoeffding Dependence Coefficients, N = 243 Prob > D under H0: D=0					
	VAR1	VAR8	VAR11	VAR12	VAR13
	0.18111	-0.00235	-0.00234	-0.00240	0.00021
coremin	<.0001	0.9977	0.9974	0.9987	0.3226

F.3   AP600: 6 inch Break, Top 5 Variables

Thursday, April 12, 2012 5:32 PM   1

Correlation Analysis

The CORR Procedure

1 With Variables:	coremin			
5 Variables:	VAR1 VAR7 VAR8 VAR12 VAR13			

SSCP Matrix					
	VAR1	VAR7	VAR8	VAR12	VAR13
coremin	12415.99854	3145.03885	6257.13615	12434.50585	3.12222

CSSCP Matrix					
	VAR1	VAR7	VAR8	VAR12	VAR13
coremin	-5.17726000	-0.00286622	46.54825000	13.33005000	-0.01413007

Covariance Matrix, DF = 242					
	VAR1	VAR7	VAR8	VAR12	VAR13
coremin	-.0213936364	-.0000118439	0.1923481405	0.0550828512	-.0000583887

Simple Statistics						
Variable	N	Mean	Std Dev	Median	Minimum	Maximum
coremin	243	51.11595	0.97550	51.09220	48.97220	53.79780
VAR1	243	1.00000	0.04091	1.00000	0.95000	1.05000
VAR7	243	0.25320	0.02072	0.25320	0.22788	0.27852
VAR8	243	0.50000	0.40909	0.50000	0	1.00000
VAR12	243	1.00000	0.24545	1.00000	0.70000	1.30000
VAR13	243	0.0002525	0.0002025	0.0002525	5E-6	0.0005000

Pearson Correlation Coefficients, N = 243 Prob > |r| under H0: Rho=0					
	VAR1	VAR7	VAR8	VAR12	VAR13
	-0.53609	-0.00059	0.48199	0.23005	-0.29558
coremin	<.0001	0.9927	<.0001	0.0003	<.0001

Spearman Correlation Coefficients, N = 243 Prob > |r| under H0: Rho=0					
	VAR1	VAR7	VAR8	VAR12	VAR13
	-0.52077	-0.00833	0.45018	0.24533	-0.30260
coremin	<.0001	0.8972	<.0001	0.0001	<.0001

Kendall Tau b Correlation Coefficients, N = 243 Prob > |tau| under H0: Tau=0					
	VAR1	VAR7	VAR8	VAR12	VAR13
	-0.41714	-0.00594	0.35799	0.19097	-0.23436
coremin	<.0001	0.9046	<.0001	0.0001	<.0001

Hoeffding Dependence Coefficients, N = 243 Prob > D under H0: D=0					
	VAR1	VAR7	VAR8	VAR12	VAR13
	0.07638	-0.00338	0.05917	0.01273	0.01938
coremin	<.0001	1.0000	<.0001	0.0010	<.0001

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F.4 AP600: 8 inch Break, Top 4 Variables

Friday, April 13, 2012 4:41 PM   1

Correlation Analysis

The CORR Procedure

1 With Variables:	coremin
4 Variables:	VAR1 VAR8 VAR12 VAR13

SSCP Matrix				
	VAR1	VAR8	VAR12	VAR13
coremin	2739.119790	1380.873250	2918.222760	0.615148

CSSCP Matrix				
	VAR1	VAR8	VAR12	VAR13
coremin	1.64289000	12.13480000	-1.75260000	-0.00078453

Covariance Matrix, DF = 80				
	VAR1	VAR8	VAR12	VAR13
coremin	0.0205361250	0.1516850000	-.0219075000	-.0000098066

Simple Statistics						
Variable	N	Mean	Std Dev	Median	Minimum	Maximum
coremin	81	33.79601	1.29386	33.96140	28.58110	37.45090
VAR1	81	1.00000	0.04108	1.00000	0.95000	1.05000
VAR8	81	0.50000	0.41079	0.50000	0	1.00000
VAR12	81	1.06667	0.23717	1.00000	0.70000	1.30000
VAR13	81	0.0002250	0.0001836	0.0002525	5E-6	0.0005000

Pearson Correlation Coefficients, N = 81 Prob > |r| under H0: Rho=0				
	VAR1	VAR8	VAR12	VAR13
	0.38637	0.28539	-0.07139	-0.04129
coremin	0.0004	0.0098	0.5265	0.7144

Spearman Correlation Coefficients, N = 81 Prob > |r| under H0: Rho=0				
	VAR1	VAR8	VAR12	VAR13
	0.32918	0.46694	-0.23755	-0.18540
coremin	0.0027	<.0001	0.0327	0.0975

Kendall Tau b Correlation Coefficients, N = 81 Prob > |tau| under H0: Tau=0				
	VAR1	VAR8	VAR12	VAR13
	0.25619	0.31788	-0.19474	-0.14414
coremin	0.0032	0.0002	0.0255	0.0983

Hoeffding Dependence Coefficients, N = 81 Prob > D under H0: D=0				
	VAR1	VAR8	VAR12	VAR13
	0.01622	0.04746	0.01046	0.00160
coremin	0.0242	0.0003	0.0588	0.2683

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F.5 LOFT: 3 Values per Variable

Correlation Analysis

The CORR Procedure

1 With Variables:	PCT					
6 Variables:	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47

SSCP Matrix

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	35809.288	3424.870	6205105.659	808202.822	681860.601	73642.606

CSSCP Matrix

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	-34.88999	-3.78793	-10562.55619	-20307.45525	-3041.22853	-2.75210

Covariance Matrix, DF = 728

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	-0.04792581	-0.00520320	-14.50900575	-27.89485611	-4.17751171	-0.00378036

Simple Statistics

Variable	N	Mean	Std Dev	Median	Minimum	Maximum
PCT	729	1010	192.24533	975.73000	723.60100	1475
VAR1	729	0.04867	0.0005781	0.04867	0.04796	0.04938
VAR25	729	0.00466	0.0000624	0.00466	0.00458	0.00473
VAR26	729	8.44000	0.68960	8.44000	7.59600	9.28400
VAR44	729	1.12500	0.30640	1.12500	0.75000	1.50000
VAR45	729	0.93000	0.15197	0.93000	0.74400	1.11600
VAR47	729	0.10000	0.04085	0.10000	0.05000	0.15000

Pearson Correlation Coefficients, N = 729
Prob > |r| under H0: Rho=0

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.43126	-0.43386	-0.10944	-0.47357	-0.14299	-0.00048
PCT	<.0001	<.0001	0.0031	<.0001	0.0001	0.9896

Spearman Correlation Coefficients, N = 729
Prob > |r| under H0: Rho=0

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.33134	-0.70081	-0.16088	-0.39616	-0.21612	0.00031
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	0.9934

Kendall Tau b Correlation Coefficients, N = 729
Prob > |tau| under H0: Tau=0

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.25922	-0.59409	-0.12552	-0.30960	-0.16669	0.00034
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	0.9906

Hoeffding Dependence Coefficients, N = 729
Prob > D under H0: D=0

	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	0.02860	0.20104	0.00631	0.04027	0.01090	-0.00119
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	1.0000

F.6   LOFT: 6 Values per Variable

Correlation Analysis

The CORR Procedure

1 With Variables:	PCT					
6 Variables:	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47

SSCP Matrix						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	741345.7	70880.1	128445869.5	16928250.1	14118361.3	1523872.0

CSSCP Matrix						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	-354.6168	-66.9270	-170739.5504	-215551.4121	-53847.9969	-21.4771

Covariance Matrix, DF = 15624						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
PCT	-0.02269692	-0.00428360	-10.92803062	-13.79617333	-3.44649237	-0.00137462

Simple Statistics						
Variable	N	Mean	Std Dev	Median	Minimum	Maximum
PCT	15625	975.29182	138.06833	960.68800	723.60100	1476
VAR1	15625	0.04867	0.0005002	0.04867	0.04796	0.04938
VAR25	15625	0.00466	0.0000540	0.00466	0.00458	0.00473
VAR26	15625	8.44000	0.59682	8.44000	7.59600	9.28400
VAR44	15625	1.12500	0.26517	1.12500	0.75000	1.50000
VAR45	15625	0.93000	0.13153	0.93000	0.74400	1.11600
VAR47	15625	0.10000	0.03536	0.10000	0.05000	0.15000

Pearson Correlation Coefficients, N = 15625 Prob > |r| under H0: Rho=0						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.32863	-0.57473	-0.13262	-0.37682	-0.18979	-0.00028
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	0.9719

Spearman Correlation Coefficients, N = 15625 Prob > |r| under H0: Rho=0						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.25152	-0.80646	-0.17079	-0.31533	-0.25236	-0.00048
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	0.9517

Kendall Tau b Correlation Coefficients, N = 15625 Prob > |tau| under H0: Tau=0						
	VAR1	VAR25	VAR26	VAR44	VAR45	VAR47
	-0.18691	-0.66938	-0.12528	-0.23445	-0.18548	-0.00035
PCT	<.0001	<.0001	<.0001	<.0001	<.0001	0.9523