Finding the Geometric Buckling Value (B_g^2) for a Practical Nuclear Reactor

MA 203 – PROJECT (2023-24)

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1. Problem Statement

To find the Geometric Buckling (B_g^2) value using the six-factor equation $k = \eta f p \epsilon P_{FNL} P_{TNL}$. The Geometric Buckling value has significance in determining the reactor's stability and safety, ensuring the nuclear fission process remains efficient while avoiding potential hazards.

1.1 Context

Nuclear reactors around the world work on the principle of nuclear fission. Nuclear fission proceeds through fission chain reaction, in which a single neutron is bombarded onto enriched Uranium isotopes such as U_{235} or U_{238}. The nucleus of these isotopes splits into two or more nuclei along with some neutrons which are utilized to continue the chain reaction. This nuclear fission reaction is controlled by a particular multiplication factor known as the effective neutron multiplication factor (k). This factor determines whether the reaction remains under control or spirals into uncontrollable territory. The basic concept of k can be expressed as:

$$k = \frac{Number\ of\ neutrons\ in\ one\ generation}{Number\ of\ neutrons\ in\ the\ preceding\ generation}$$

However, real-world nuclear reactors are influenced by a myriad of complex factors. To account for these complexities, we employ the six-factor formula to calculate k.

1.2 Theory

- Geometric Buckling (B_g^2) is a specific way of measuring how neutrons behave within the reactor's geometry (shape and size). It's like a mathematical quantity that tells us how confined the neutrons are inside the reactor. If B_g^2 is too small, neutrons escape too easily, and the reactor won't work efficiently. If it's too big, the reactor might become unstable.
- It is a simple Helmholtz eigenvalue problem that is solved for different geometries.
- The buckling value is crucial for determining the spatial behavior of neutron flux within the reactor, affecting how neutrons interact with fissile material and influencing the multiplication factor.
- It considers the curvature of neutron flux and describes how the neutron population changes as a function of distance within the reactor.
- In practical terms, engineers and physicists use B_g^2 to design safe and efficient reactors. They adjust the reactor's size, shape, and materials used to achieve the right balance of neutron confinement. This helps ensure that the reactor operates smoothly and doesn't pose a risk.

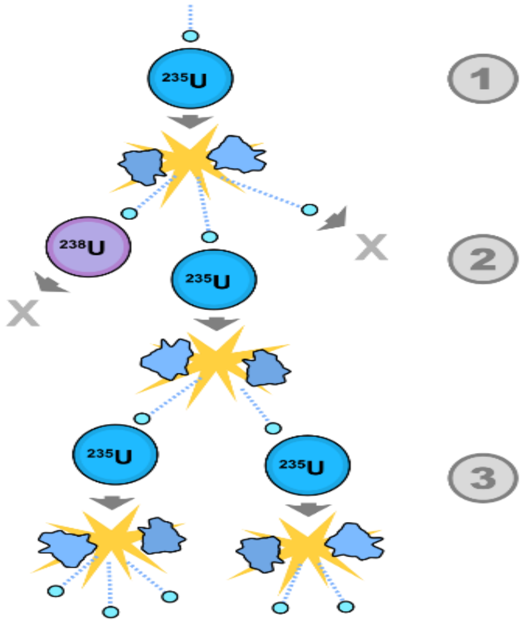

Fig. 1 Nuclear fission chain reaction [source: Wikipedia]

1.3 Approach

- Implement an appropriate numerical method to find the value of geometrical buckling with *good accuracy*.
- Develop *test cases* with known solutions to validate our computed results.
- Explore *multiple methods* (open and bracket methods) to improve algorithm efficiency.
- Try implementing the algorithm in *different programming languages* to get a more precise value.
- Investigate how *changes in input parameters* impact the calculated value.

2. Physical model

The fundamental principle behind a nuclear reactor is to convert the heat generated by nuclear fission into electricity through a series of interconnected processes. By controlling factors like the position of control rods and the coolant flow, operators manage the reactor's power output.

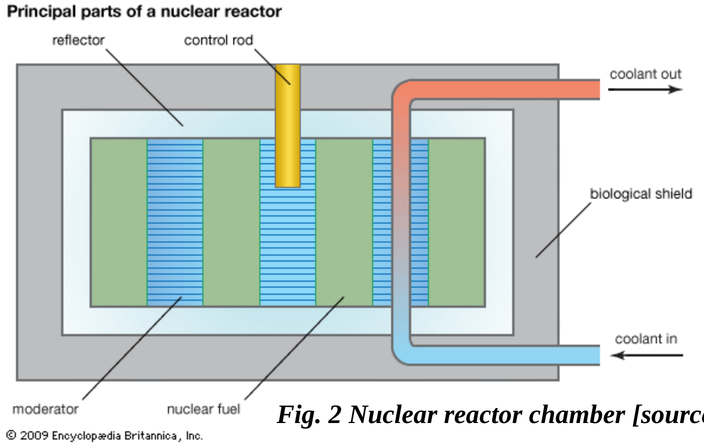

Fig. 2 Nuclear reactor chamber [source: Britannica]

A nuclear reactor functions by orchestrating a controlled nuclear fission process. Initially, nuclear fuel, typically enriched Uranium-235 or Plutonium-239, is prepared and formed into fuel rods or pellets. Control rods, which can absorb neutrons and regulate the reaction rate, are inserted into the core. A moderator, such as water or graphite, is employed to slow down fast neutrons, increasing their probability of triggering further fission. A coolant circulates through the core, extracting heat produced during fission. In the core, neutrons initiate fission reactions when they collide with fissile nuclei, releasing substantial heat energy. This heat is transferred to the coolant, which is used to produce steam. The high-pressure steam propels a turbine, connected to an electrical generator, producing electricity.

3. Assumptions

The following assumptions have been made in the six-factor-formula and in the assumed typical values of the different parameters in the formula.

1. **Standard Temperature and Pressure (STP):** Thermal values are often given under standard temperature and pressure conditions, which are 0 degrees Celsius (273.15 Kelvin) and 1 atmosphere of pressure (101.3 kPa). This standardizes the values for comparison purposes.

2. **Pure Materials:** Thermal values are typically given for pure materials, assuming that the materials are not impure or mixed with other substances. Impurities can significantly affect thermal properties, so pure materials are assumed for standard values.

3. **Homogeneous and Isotropic Materials:** The materials are assumed to be homogeneous (having uniform composition throughout) and isotropic (having the same thermal properties in all directions). Materials in a reactor might have complex structures, but for standard values, simplicity is assumed.

4. **Moderators:** Usually we use heavy water in modern reactors, but instead we have chosen a different approach to solve for the earlier 20th century reactors. So, the moderators which we have considered are made up of graphite which influences a lot of variables in the upcoming equations, such as fermi age of neutrons (τ_{th}) and diffusion length of thermal neutrons (${L_{th}}^2$).

Symbol	Name	Typical thermal reactor value
η	Thermal fission factor (eta)	1.65
f	Thermal utilization factor	0.71
p	Resonance escape probability	0.87
ϵ	Fast fission factor (epsilon)	1.02
P_{FNL}	Fast non-leakage probability	0.97
P_{TNL}	Thermal non-leakage probability	0.99

4. Governing Equations

The mathematical idea we have described in our problem statement is governed by the following set of equations:

4.1 Six Factor Equation

$$k = \eta f p \epsilon P_{FNL} P_{TNL} \quad (1)$$

$$P_{FNL} \approx \exp\left(-{B_g}^2 \tau_{th}\right) \quad (1.1)$$

$$P_{TNL} \approx \frac{1}{1 + {L_{th}}^2 {B_g}^2} \quad (1.2)$$

The six-factor equation is a neutron life-cycle balance equation that is used in nuclear engineering to determine the multiplication of a nuclear chain reaction in a non-infinite medium. It is a complex equation that considers several factors, including the number of neutrons produced per fission, the probability of neutrons being absorbed or scattered, and the probability of neutrons leaking out of the reactor.

Where:

- k is the effective multiplication factor, which is a measure of the rate of growth of the neutron population.
- ϵ is the fast fission factor, which is the ratio of the number of neutrons produced from fast fissions to the number of neutrons produced from thermal fissions.
- L is the fast non-leakage factor, which is the probability that a fast neutron will not leak out of the reactor before it undergoes fission.
- f is the thermal fuel utilization factor, which is the fraction of thermal neutrons that are absorbed in the fuel.
- p is the resonance escape probability.
- η is the thermal fission factor, which is the average number of neutrons produced per fission.
- P_{FNL} is the fast non-leakage probability.
- P_{TNL} is the thermal non-leakage probability.
- ${B_g}^2$ is the geometric buckling.
- ${L_{th}}^2$ is the diffusion length of thermal neutrons.
- τ_{th} is the fermi age of neutron.

$$k = \eta f p \epsilon e^{-B_g^2 \tau_{th}} \frac{1}{1 + L_{th}^2 B_g^2} \quad (1.3)$$

- If k is greater than 1, the chain reaction is *supercritical*, and the neutron population will grow exponentially.
- If k is less than 1, the chain reaction is *subcritical*, and the neutron population will exponentially decay. **This is the condition we aim to solve for in this project.**
- If k = 1, the chain reaction is *critical*, and the neutron population will remain constant.

$$\eta f p \epsilon e^{-B_g^2 \tau_{th}} \frac{1}{1 + L_{th}^2 B_g^2} = 0.99 \quad (2)$$

5. Boundary Conditions

5.1 Physical Boundary Conditions

- The **temperature range** for a nuclear fission reaction in a typical nuclear reactor is in the range of **600°C to 1000°C**. Nuclear fission requires a critical mass of fissile material to sustain a chain reaction, and the temperature affects the density and geometry of the material. Thus, the temperature must be in the above range to prevent an explosion or a meltdown of the nuclear reactor.

- The **critical mass**, which is the minimum amount of fissile material that can sustain a chain reaction, depends on the type of fissile material, its shape, density, purity, and temperature. So, the critical mass of:
  - Uranium-235: **50 kilograms** (without a reflector) [1]
  - Plutonium-239: **10 kilograms** (without a reflector) [1]
  - Thorium-233: **11 kilograms** (without a reflector) [1]

- There is **a minimum energy requirement for the incident neutron** (neutron which bombards the nucleus) to make sure it bombards the nucleus of the fissile isotope and sustains the fission chain reaction. This depends on the fissile material and the number of neutrons present in its nucleus. [1]
  - For even number of neutrons: **Energy ≥ 1 MeV**
  - For odd number of neutrons: **Fission can occur with thermal (slow) neutrons.**

5.2 Boundary conditions of geometric buckling B_g^2 in numerical methods used

The boundary conditions for geometric buckling ${B_g}^2$ can be observed once we plot the equation (2).

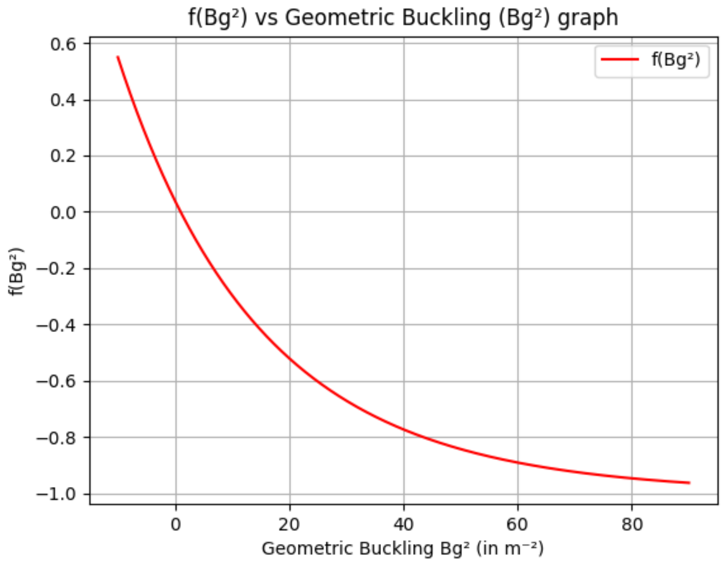

Fig. 3 Graph of the equation (2)

From Fig. 1 we can see what range we could take as the lower boundary and upper boundary of geometric buckling ${B_g}^2$ in the numerical methods performed below.

- **Bracketing methods:**
  - The bisection method: $\boldsymbol{B^2_{g}}_{\boldsymbol{lowest}}$ = *-10* and $\boldsymbol{B_{g^2}}_{\boldsymbol{highest}}$ = *10*
  - The false-position method: $\boldsymbol{B^2_{g}}_{\boldsymbol{lowest}}$ = *-5* and $\boldsymbol{B_{g^2}}_{\boldsymbol{highest}}$ = *5*

- **Open methods:**
  - Simple fixed-point iteration: $\boldsymbol{B_{g^2}}_{\boldsymbol{0}}$ = *5*, as the algorithm will converge to the root.
  - The Newton-Raphson method: $\boldsymbol{B_{g^2}}_{\boldsymbol{0}}$ = *-100*

6. Parameters

The **parameters in the equation (2)** are used to perform numerical methods on it. Now let's define and assign some typical values (in real life nuclear reactors) to these parameters.

6.1 Thermal fission factor (η)

The thermal fission factor (η), is one of six factors that affect how a nuclear chain reaction sustains itself. It measures how many neutrons from thermal fission cause more fissions, compared to how many thermal neutrons the fuel absorbs. The fuel type, enrichment, and average neutrons per fission influence this factor.

$$\eta = \frac{neutrons\ produced\ from\ fission}{absorption\ in\ fuel\ isotope}$$

The typical value of $\boldsymbol{\eta}$ used in real life nuclear reactors is **1.65**, so in equation (2) we substitute this value [1].

6.2 Thermal utilization factor (f)

The thermal utilization factor in a nuclear reaction is a measure of how well the thermal neutrons are used to cause fission in the fuel. It is the ratio of the thermal neutrons absorbed by the fuel to the thermal neutrons absorbed by any material in the reactor core.

$$f = \frac{neutrons\ absorbed\ by\ the\ fuel\ isotope}{neutrons\ absorbed\ anywhere}$$

The typical value of $\boldsymbol{f}$ used in real life nuclear reactors is **1.65**, so in equation (2) we substitute this value [1].

6.3 Resonance escape probability (p)

Resonance escape probability is how likely a neutron can avoid being absorbed by a non-fissile nucleus as it loses energy. This absorption would make the neutron useless and lower the chain reaction. Resonance escape probability varies with the fuel type, the core shape and layout, and the neutron energy. Resonance escape probability is one of the factors that influence how a nuclear chain reaction keeps going.

$$p = \frac{fission\ neutrons\ slowed\ to\ thermal\ energies\ without\ absorption}{total\ fission\ neutrons}$$

The typical value of $\boldsymbol{p}$ used in real life nuclear reactors is **0.87**, so in equation (2) we substitute this value [1].

6.4 Fast fission factor (ϵ)

Fast fission factor is a measure of how many neutrons are produced by fission at any energy level, compared to how many neutrons are produced by fission at thermal energy level. Fast fission factor is influenced by the type and arrangement of the fuel and the moderator, because they affect the neutron flux spectrum.

$$\epsilon = \frac{total\ number\ of\ fission\ neutrons}{number\ of\ fission\ neutrons\ from\ just\ thermal\ fissions}$$

The typical value of $\boldsymbol{\epsilon}$ used in real life nuclear reactors is **1.02**, so in equation (2) we substitute this value [1].

6.5 Fermi age of neutrons (τ_{th})

Fermi age of neutron in nuclear reactions is a concept that measures how far a neutron travels in a moderator, such as graphite, before it slows down to thermal energy. It is called “age” because the neutron lifetime is proportional to how long it takes to slow down. Fermi age is one of the factors that affect how a nuclear chain reaction sustains itself.

In our case, we have assumed fermi age of neutrons in a particular moderator i.e., graphite. So, when we take moderator as **graphite**, the $\boldsymbol{\tau_{th}}$ would be **0.03 $\mathbf{m^2}$** (conventionally measured in m^2 even though we are defining it in length) [1].

6.6 Diffusion length of thermal neutrons ($L_{th}{}^2$)

Diffusion length of thermal neutrons is a quantity that shows how much distance a neutron covers in a material before it gets absorbed. It is obtained by dividing the diffusion coefficient, which indicates how well neutrons spread in the material, by the absorption cross-section, which indicates how probable neutrons are trapped by nuclei. Diffusion length of thermal neutrons varies with the kind and mixture of the moderator, and it influences the neutron flow pattern and the reactivity of a nuclear reactor.

In our case, since we have taken moderator as **graphite**, the value of $\boldsymbol{L_{th}{}^2}$ is approximately equal to **0.0094009 $\mathbf{m^{-2}}$** [1].

7. Analytical Solution Methodology

Analytical solution for our above-mentioned solution is as follows:

$$k = \eta f p \epsilon e^{-B_g^2 \tau_{th}} \frac{1}{1 + L_{th}^2 B_g^2}$$

Our aim is to find the value of $-B_g^2$ in the above equation for $k < 1$. Let B_g^2 be x.
Then our equation becomes:

$$\eta \cdot f \cdot p \cdot \epsilon \cdot e^{-x\tau_{th}} \cdot \frac{1}{1 + L_{th}^2 x} = 0.99 \tag{3}$$

where,

$f = 0.71$
$\tau_{th} = 0.03\ m^2$
$\eta = 1.65$
$L_{th}^2 = 0.0094009\ /m^2$
$\epsilon = 1.02$
$p = 0.87$

$$1.65 \cdot 0.71 \cdot 0.87 \cdot 1.02 \cdot e^{-x \cdot 0.03} \frac{1}{1 + 0.0094009x} = 0.99$$

$$1.0395891 e^{-x \cdot 0.03} = (1 + 0.0094009x)0.99$$

$$e^{-x \cdot 0.03} = 0.9522993 + 0.0089524\text{x}$$

$$x \cdot 0.03 = \ln\left(\frac{1}{0.9522993 + 0.0089524x}\right)$$

Now this equation cannot be solved by conventional methods. Below are the solutions for the same using numerical methods.

8. Algorithms used for Numerical Methods

8.1 Bisection Method – Bracketing Method

The bisection method is a numerical technique used for finding the root of a real-valued function within a specified interval. It is an iterative method based on the intermediate value theorem, which states that if a continuous function changes sign over an interval, then it must have at least one root in that interval.

This method consists of four parts as shown below.

i. **Initialization:**
   - Choose an interval [a, b] where the function changes sign.
   - Verify that the function is continuous on the interval.

ii. **Iteration:**
   - Calculate the midpoint, c, of the interval: $c = \frac{a+b}{2}$
   - Evaluate the function at c.
   - Determine the new interval [a, c] or [c, b] based on the sign of the function at c.
   - Repeat the process until a satisfactory approximation of the root is achieved or a convergence criterion is met.

iii. **Convergence Criteria:**
   - Stop the iteration when the width of the interval is smaller than a predetermined tolerance.
   - Alternatively, terminate when the function value at the midpoint is close to zero.

iv. **Result:**
   - The final midpoint or any value within the final interval is an approximate root of the function.

The bisection method is guaranteed to converge to a root because it continually refines the interval where the root is located. However, it may converge slowly compared to some other methods.

8.2 False-Position Method – Bracketing Method

The False Position Method, also called the Regula Falsi method, is a numerical approach to approximate roots of nonlinear equations. It starts with two initial guesses, x_l and, x_u, ensuring opposite signs for $f(x_l)$ and $f(x_u)$. Through iterative refinement using linear interpolation, it converges to the root within a chosen interval.

This method consists of the following parts:

i. **Initialization:**
   - Choose two initial guesses, x_l and x_u, such that $f(x_l)$ and $f(x_u)$ have opposite signs. This ensures that there is a root of the function within the interval $[x_l, x_u]$.
   - Ensure that the function is continuous and differentiable in the neighbourhood of the initial guess.

ii. **Iteration:**

- At each iteration n, calculate the next approximation x_{n+1}, using the formula: $x_{n+1} = x_n - \frac{f(x_n).(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})}$
  where $f(x_n)$ is the function value at x_n.

iii. **Convergence Criteria:**

- Calculate $f(x_{n+1})$
- If $f(x_{n+1}) = 0$ (i.e., you've found the root), or if $f(x_{n+1})$ is smaller than a predetermined tolerance, you can proceed to the result and stop the iteration.

iv. **Result:**

- The final x_{n+1} value is an approximate root of the function.

This method is suitable for continuous functions with a single root, though convergence may be slow for certain functions or fail in some cases.

8.3 Simple Fixed-Point Iteration Method – Open Method

The Fixed-Point Iteration Method is a numerical technique for approximating roots of equations. It involves transforming the equation into the form $x = g(x)$, selecting an initial guess, x_0, and iteratively applying $g(x)$ to find successive approximations. Convergence depends on $|g'(x)| < 1$ near the root but isn't assured for all functions or guesses.

This method consists of the following parts:

i. **Initialization:**

- Convert the equation $f(x) = 0$ into the form $x = g(x)$ to establish a fixed-point iteration.

ii. **Iteration:**

- Start with an initial guess x_0 close to the root.
- Iteratively update the guess using the function $g(x)$: $x_{n+1} = g(x_n)$

iii. **Convergence Criteria:**

- Calculate the $Stopping\ criterion = \frac{x_{n+1} - x_n}{x_{n+1}}$.
- If the $Stopping\ criterion$ is near 0 or if it is less than your specified value (depending on the accuracy) you can stop the iteration.

iv. **Result:**

- The final x_{n+1} value is an approximate root of the function.

It is to be noted that the method's success depends on factors like the choice of $g(x)$ and the initial guess, and it may not always converge, especially if $|g'(x)| \geq 1$ near the root or if $g(x)$ does not meet the conditions for convergence.

8.4 Newton-Raphson Method – Open Method

The Newton-Raphson method, also known as the Newton method, is a numerical technique used for finding the roots of a real-valued function. It's an iterative method that starts with an initial guess and refines the estimate through successive iterations. The method is based on linear approximation and employs the derivative of the function.

This method consists of the following parts:

i. **Initialization:**
   - Choose an initial guess x_0, close to the actual root.
   - Ensure that the function is continuous and differentiable in the neighbourhood of the initial guess.

ii. **Iteration:**
   - At each iteration n, calculate the next approximation x_{n+1}, using the formula: $x_{n+1} = x_n - \frac{f(n)}{f'(n)}$
     where $f(x_n)$ is the function value at x_n, and $f'(x_n)$ is the derivative of the function evaluated at x_n.

iii. **Convergence Criteria:**
   - Stop the iteration when the change in the values of x between successive iterations is sufficiently small.
   - Alternatively, stop if the function value is close to zero.

iv. **Result:**
   - The final x value is an approximate root of the function.

The Newton-Raphson method often converges rapidly when the initial guess is close to the true root, especially for well-behaved functions. However, it may fail to converge or converge to a different root if the initial guess is far from the actual root or if the function has certain characteristics (e.g., flat regions, vertical asymptotes) that impede convergence.

9. Results and Observations

9.1 Bisection Method – Bracketing Method

On taking the boundary condition $\boldsymbol{B^2_{g}}_{\boldsymbol{lowest}}$ = ***-10*** & $\boldsymbol{B^2_{g}}_{\boldsymbol{highest}}$ = ***10,*** we obtain the $\boldsymbol{B^2_g}$ converging at a value of **1.2392330766149917 m⁻².** The graph shown below depicts the convergence of $\boldsymbol{B^2_g}$ with respect to the number of iterations.

```
base ~/Documents/Python (25.97s)
python bisection.py
Bisection Method:

The Geometric Buckling Value (Bg^2) is approximately 1.2392330766149917 m^-2

The corresponding f(Bg^2) Value is 0.0
```

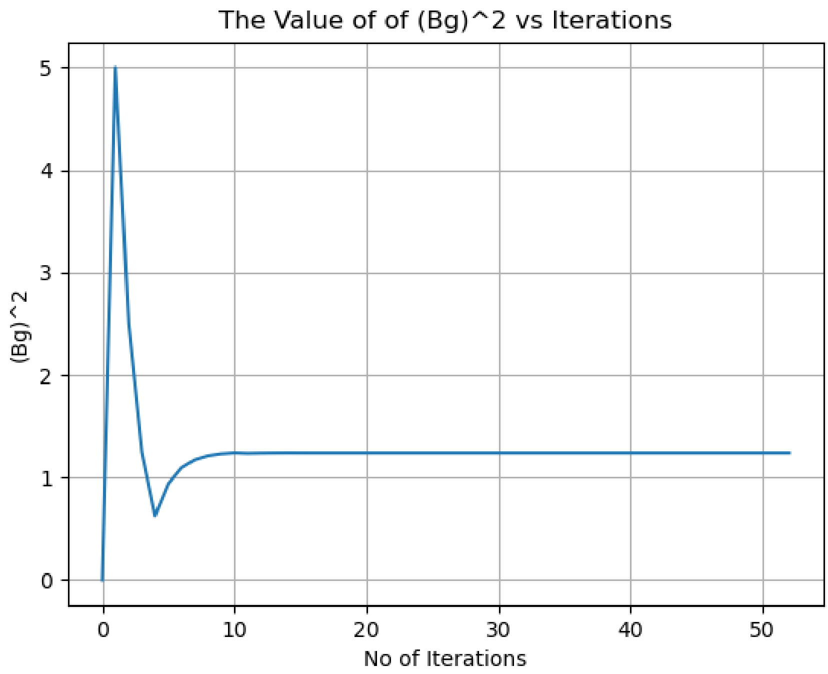

Fig. 4 Graph depicting the variation of B_g^2 with respect to the number of iterations calculated using Bisection

9.2 False-Position Method – Bracketing Method

On taking the boundary condition $B^2_{g\,lowest}$ = *-5* & $B^2_{g\,highest}$ = *5,* we obtain the B_g^2 converging at a value of **1. 2421932859905613 m⁻².** The graph shown below depicts the convergence of B_g^2 with respect to the number of iterations.

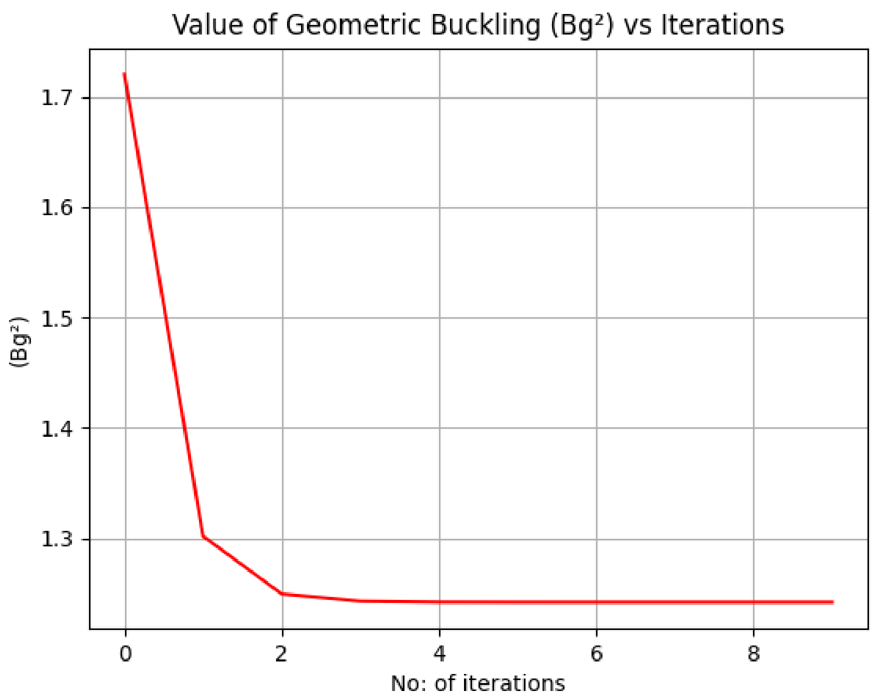

Fig. 5 Graph depicting the variation of B_a^2 with respect to the number of iterations calculated using False Position

```
False-Position Method:

The Geometric Buckling (Bg²) is approximately 1.2421932859905613 m⁻²

For verification we can see f(Bg²) is -1.3574796842164005e-10

[Finished in 1.8s]
```

9.3 Simple Fixed-Point Iteration Method – Open Method

On taking the base condition $\boldsymbol{B_{g^2}}_{\boldsymbol{0}} = \mathbf{5}$, we obtain the $\boldsymbol{B_g^2}$ converging at a value of **1.242193284032208 m⁻².** The graph shown below depicts the convergence of $\boldsymbol{B_g^2}$ with respect to the number of iterations.

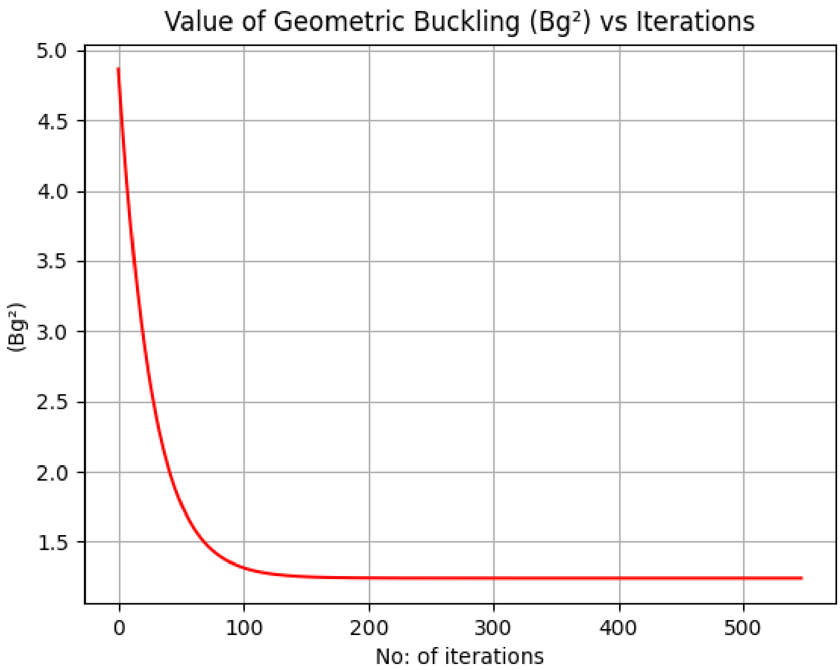

Fig. 6 Graph depicting the variation of $\boldsymbol{B_g^2}$ with respect to the number of iterations calculated using Fixed Point Iteration method.

```
Simple Fixed-Point Iteration Method:

The Geometric Buckling (Bg²) is approximately 1.242193284032208 m⁻²

For verification we can see f(Bg²) is -4.989577672643144e-11

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```

9.4 Newton-Raphson Method – Open Method

On taking the base condition $\boldsymbol{B_{g^2}}_{\boldsymbol{0}} = \mathbf{-100}$, we obtain the $\boldsymbol{B_g^2}$ converging at a value of **1.239233076614992 m⁻²**. The graph shown below depicts the convergence of $\boldsymbol{B_g^2}$ with respect to the number of iterations.

```
base ~/Documents/Python (3.706s)
python newton.py
Newton-Raphson Method:

The Geometric Buckling Value (Bg^2) is approximately 1.239233076614992 m^-2

The corresponding f(Bg^2) Value is 0.0
```

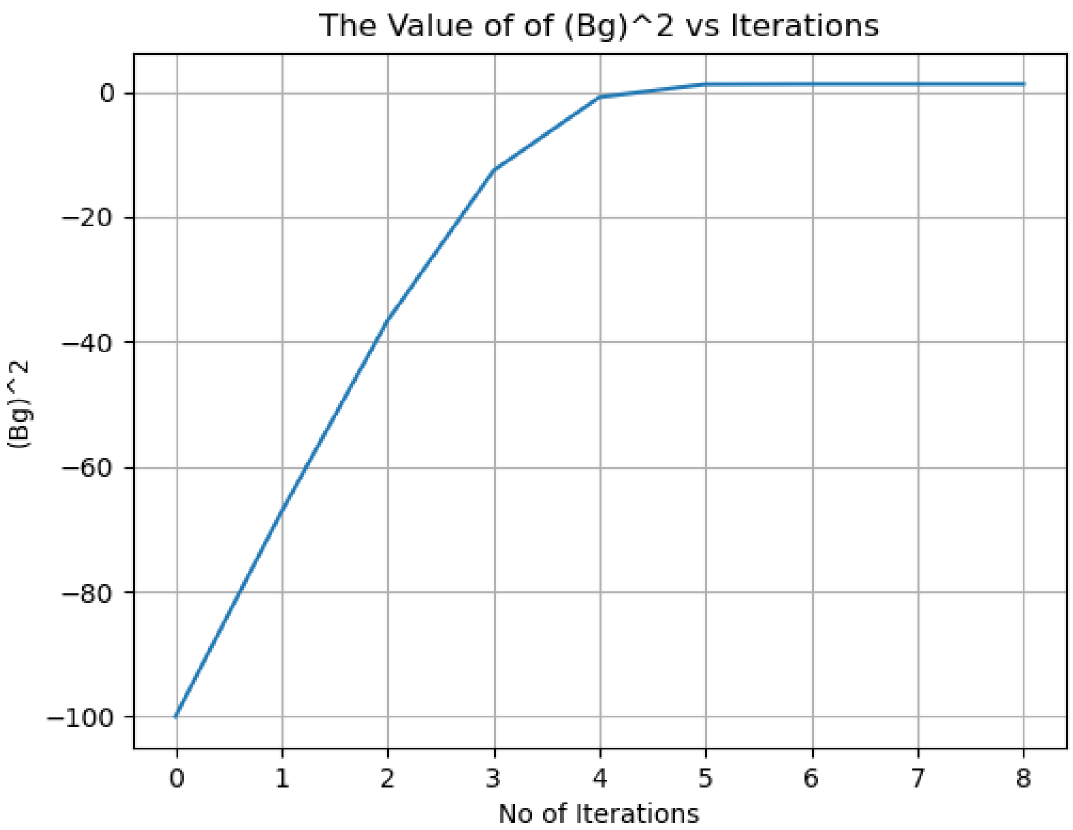

Fig. 7 Graph depicting the variation of $\boldsymbol{B_g^2}$ with respect to the number of iterations calculated using Newton-Raphson method.

As we can see from the results and the graphs the most precise value of geometric buckling $(B_g)^2$, would be the average of all values obtained from the four numerical methods. Hence,

$$(B_g)^2 = \frac{(result)_{10.1} + (result)_{10.2} + (result)_{10.3} + (result)_{10.4}}{4}$$

$$(B_g)^2 = \frac{(1.239233076614992 + 1.239233076614992 + 1.242193284032208 + 1.242193284032208)}{4}$$

$$(B_g)^2 = 1.24071318\ m^{-2}$$

Therefore, the value of $\left(B_g\right)^2$is found through four numerical methods is bound to produce a very accurate answer to our problem. Now, let's check the credibility of the geometric buckling value by substituting it in equation (2):

$$\eta f p \epsilon e^{-B_g^2 \tau_{th}} \frac{1}{1 + L_{th}^2 B_g^2} = 0.99$$

$$1.65 \cdot 0.71 \cdot 0.87 \cdot 1.02 \cdot e^{-(1.24071318) \cdot 0.03} \frac{1}{1 + 0.0094009.(1.24071318)} = 0.99$$

$$0.9900576 \approx 0.99$$

Thus, we have clearly verified that value of geometric buckling $\left(B_g\right)^2$ is very accurate from the above LHS = RHS equation.

Therefore, a geometric buckling $\boldsymbol{\left(B_g\right)^2}$of **1.24071318 m⁻²** is required to produce a multiplication factor ***(k)*** of 0.990576, which is less than 1 and makes the chain reaction **subcritical**, neutron population will exponentially decay. **This is the condition we are required to meet to sustain a chain reaction in a real-life nuclear reactor.**

10. References

[1] "Nuclear fission chain reaction: Definition," Nuclear Power, https://www.nuclear-power.com/nuclear-power/reactor-physics/nuclear-fission-chain-reaction/ (accessed Oct. 3, 2023).