# STIFF SYSTEMS ASSOCIATED WITH THE RADIOISOTOPES PRODUCTION

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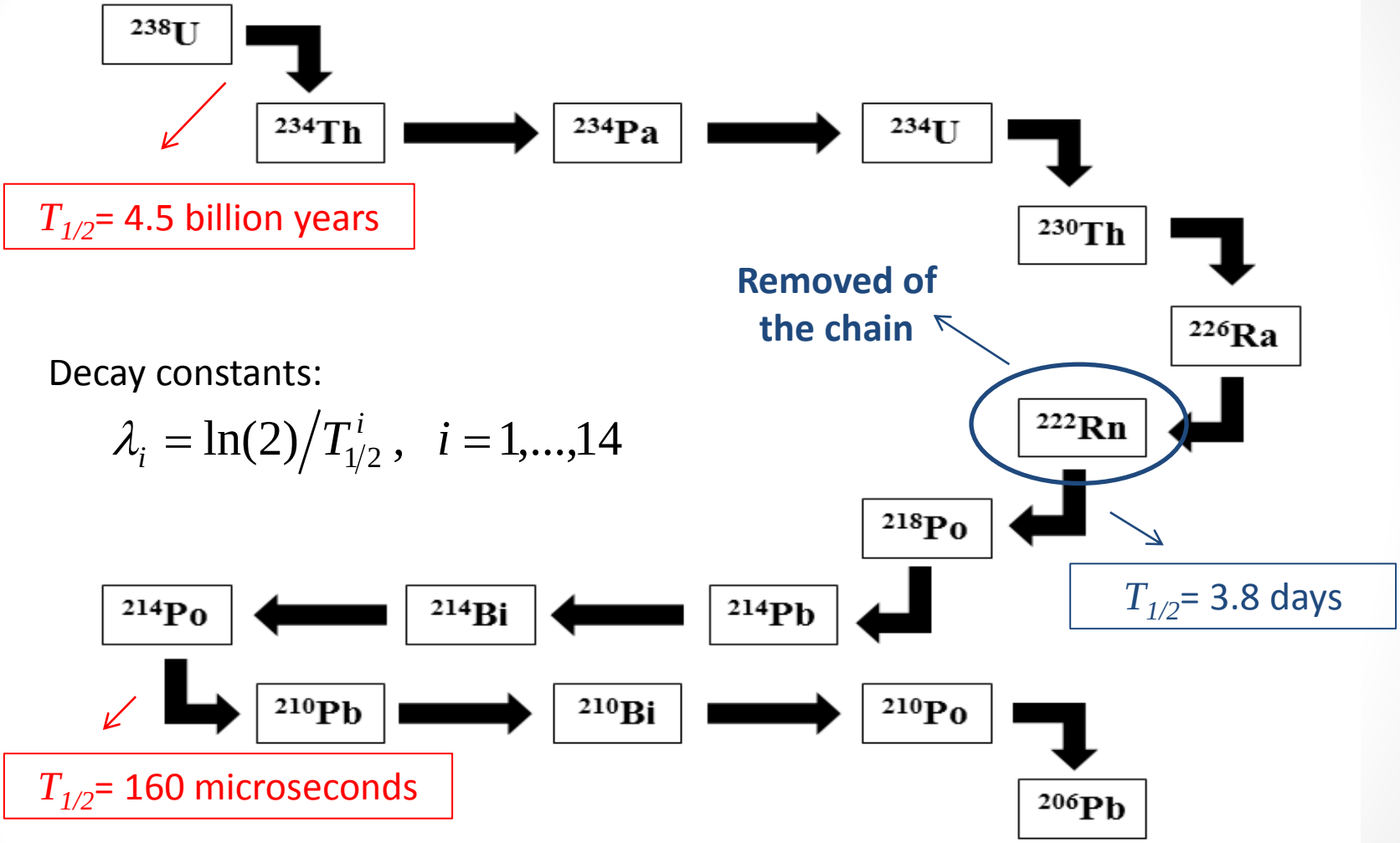
# Benefits of Nuclear Techniques

- Industry;
- Agriculture;
- Medicine:
  - sterilization of surgical materials;
  - diagnosis and treatment of diseases (scintigraphy, radiography and radiotherapy).
- The main medically useful radioisotopes are produced in particle accelerators and in nuclear reactors where occurs the radioactive decay chains.

# The Problem: Natural Decay of Uranium-238




Decay constants:

$$\lambda_i = \ln(2)/T_{1/2}^i, \quad i = 1,\ldots,14$$

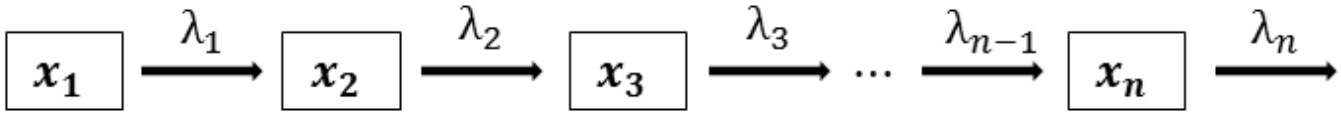
# The Problem: Natural Decay of Uranium-238

Half-lives and decay constants of the natural decay series of $^{238}U$

| Element | Variable $x_i$ | Half-Life | Decay Constant $\lambda_i$ (day$^{-1}$) |
|---|---|---|---|
| $^{238}U$ | $x_1$ | 4.5 billion years | 0.000000000000422007 |
| $^{234}Th$ | $x_2$ | 24 days | 0.028881132523331060 |
| $^{234}Pa$ | $x_3$ | 1.2 minutes | 831.7766166719343000 |
| $^{234}U$ | $x_4$ | 240000 years | 0.000000007912639047 |
| $^{230}Th$ | $x_5$ | 77000 years | 0.000000024662771057 |
| $^{226}Ra$ | $x_6$ | 1600 years | 0.000001186895857123 |
| $^{222}Rn$ | $x_7$ | 3.8 days | 0.182407152778933000 |
| $^{218}Po$ | $x_8$ | 3.1 minutes | 321.9780451633295000 |
| $^{214}Pb$ | $x_9$ | 27 minutes | 36.96784962986375000 |
| $^{214}Bi$ | $x_{10}$ | 20 minutes | 49.90659700031606000 |
| $^{214}Po$ | $x_{11}$ | 160 microseconds | 374299477.5023704000 |
| $^{210}Pb$ | $x_{12}$ | 22 years | 0.000086319698699869 |
| $^{210}Bi$ | $x_{13}$ | 5 days | 0.138629436111989100 |
| $^{210}Po$ | $x_{14}$ | 140 days | 0.004951051289713895 |

# Modeling

- The simplest model for the radioactive decay series is a first order linear system of ordinary differential equations (ODEs) with constant coefficients:




$$\lambda_i > 0, i = 1,\ldots,n$$

$$\begin{cases} x'(t) = A \cdot x(t) \\ x(0) = x_0 \end{cases}$$

being $t \in [t_0, +\infty[$, the components of the vector $x(t)$ representing the amount of each element in the chain, the initial conditions given by $x_0 = \begin{pmatrix} x_0^1 & x_0^2 & \cdots & x_0^n \end{pmatrix}^T$ and the coefficients matrix $A$ composed by the decay constants of the elements.

# Modeling

- *Stiffness* is usual in this kind of system because of the large difference in the order of the magnitudes of the decay constants which causes some of the components of the solution to decay more rapidly than others.

- A linear system with constant coefficients is *stiff* when all eigenvalues of the coefficients matrix $A$, $\lambda_i, i = 1,\ldots,n$, have real part $\mathrm{Re}(\lambda_i) > 0$ and the *stiffness ratio* $\alpha$ given by:

$$\alpha = \frac{\max\limits_{1\le i\le n}\left|\mathrm{Re}(\lambda_i)\right|}{\min\limits_{1\le i\le n}\left|\mathrm{Re}(\lambda_i)\right|},$$

  is very large.

  - Stiffness ratio: $10^{20}$
  - Determinant: $8.7353\times10^{-27}$

# Objectives

- The mathematical goal of this work is to guarantee a consistent, precise and stable numerical solution for stiff problems using Rosenbrock algorithm.

- The objective in the nuclear area is to estimate the radioactive waste generated after the removal of an amount of a chain element.

# Numerical Solutions

- Independent of the existence of analytical solutions, changes in the model or adjustments of data are easily treated by numerical methods.

- Stiff systems usually generate numerical instabilities requiring caution in the choice of the numerical method. Implicit methods like Rosenbrock and BDF (Backward Differentiation Formulae) have much higher performance than the explicit methods as Runge-Kutta Class.

- In general a very small integration step is required to maintain the stability of explicit algorithms generating very slow simulations.

# Rosenbrock Algorithm

- The Rosenbrock methods are also known as Runge-Kutta linearly implicit methods.
- They are single-step methods constructed as an alternative to solve implicit equations.
- The main idea is to solve a sequence of linear systems instead of solving nonlinear systems.

# Rosenbrock Algorithm

- ODE: $\begin{cases} x'(t) = f(x(t)) \\ x(t_0) = x_0 \end{cases}$
- A *s-stage Rosenbrock method*:

$$x_{n+1} = x_n + \sum_{j=1}^{s} b_j \kappa_j$$

Integration step — Correction of the previous solution — Linear combination of the derivatives with respect to each component of $x$

$$\kappa_i = h\,[\, f(x_n + y_n) + J\,u_n \,], \qquad i = 1, \ldots, s$$

$$y_n = \sum_{j=1}^{i-1} \alpha_{ij} \kappa_j \qquad u_n = \sum_{j=1}^{i-1} \gamma_{ij} \kappa_j + \gamma_{ii} \kappa_i \longrightarrow \text{Implicit term}$$

where $\alpha_{ij}$, $\gamma_{ij}$, $b_j$ are coefficients determined according to the desired order of consistency and stability, $h$ is the integration step and $J = f'(x_n)$ is the Jacobian matrix of the system.

# Rosenbrock Algorithm

- Each stage of this method consists of a system of linear equations with unknowns $\kappa_i$ and with matrix $I - h\gamma_{ii}J$.

- Of special interest are methods for which $\gamma_{11} = \cdots = \gamma_{ss} = \gamma$, so that we need only one LU-decomposition per step.

- The matrix-vector multiplication $J\sum \gamma_{ii}\kappa_j$ that appears in each stage can be avoided by introducing new variables:

$$u_i = \sum_{j=1}^{i} \gamma_{ij}\kappa_j, \quad i = 1, \ldots, s$$

# Rosenbrock Algorithm

- Since the Rosenbrock methods are single step methods they have the facility to change the size of the integration step automatically. The control step size is based on formulas that use embedded vectors already calculated.

- The Rosenbrock method implemented for this work is a 3rd-order and 4-stages method using the change of variables described above to reduce computational spending.

- A 2nd-order embedded formula is used to control the size of the integration step.

# Rosenbrock Algorithm

$$\begin{cases} x_0 = x(t_0) \\ x^*_{n+1} = x_n + 2u_1 + u_3 \quad \text{and} \quad x_{n+1} = x_n + 2u_1 + u_3 + u_4 \end{cases}$$

Where $u_1, u_2, u_3$ and $u_4$ are solutions of the following linear systems:

$$\left(\frac{2}{h}I - J\right)u_1 = f(x_n),$$

$$\left(\frac{2}{h}I - J\right)u_2 = f(x_n) + \frac{4}{h}u_1,$$

$$\left(\frac{2}{h}I - J\right)u_3 = f(x_n + 2u_1) + \frac{1}{h}u_1 - \frac{1}{h}u_2,$$

$$\left(\frac{2}{h}I - J\right)u_4 = f(x_n + 2u_1 + u_3) + \frac{1}{h}u_1 - \frac{1}{h}u_2 - \frac{8}{3h}u_3.$$

$$h_0 \leq \left(\frac{120\varepsilon}{t_f \left\|A^5\right\|_1 \left\|x_0\right\|_1}\right)^{1/4}$$

$\varepsilon = 10^{-04}$ and $h_0 = 10^{-15}$

The algorithm was implemented in Fortran 90 and was run on a machine with Intel® Core™ i5 processor and Windows® 7 64-bit.

# Results

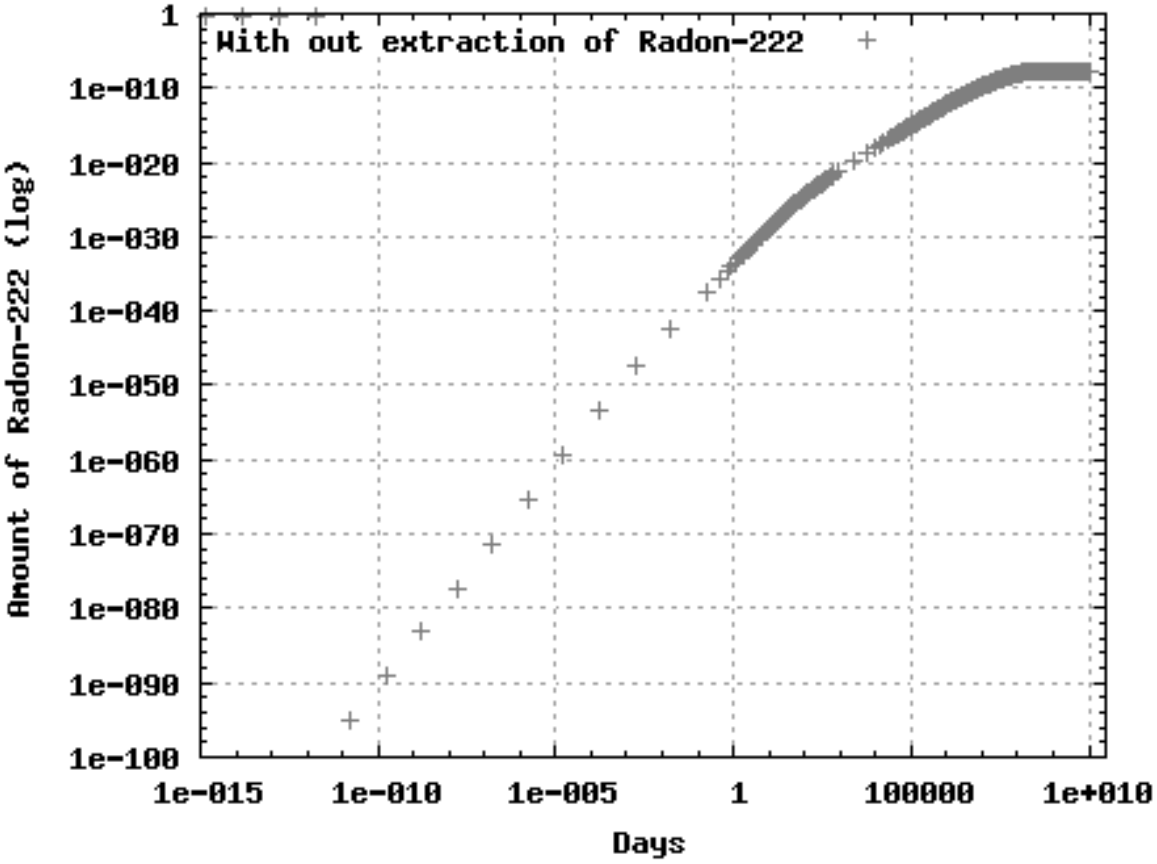
- Initial Conditions:
  - $x_0$ : $10^{04}$ units of $^{238}U$ and the inventory of the other elements of the series is zero
  - $t_f$ : 10 billion days

- CASE 1: the natural decay series of Uranium-238

- CASE 2: assuming that 10% of the $^{222}Rn$ produced is continuously removed from the sample during the process of natural decay series of Uranium-238

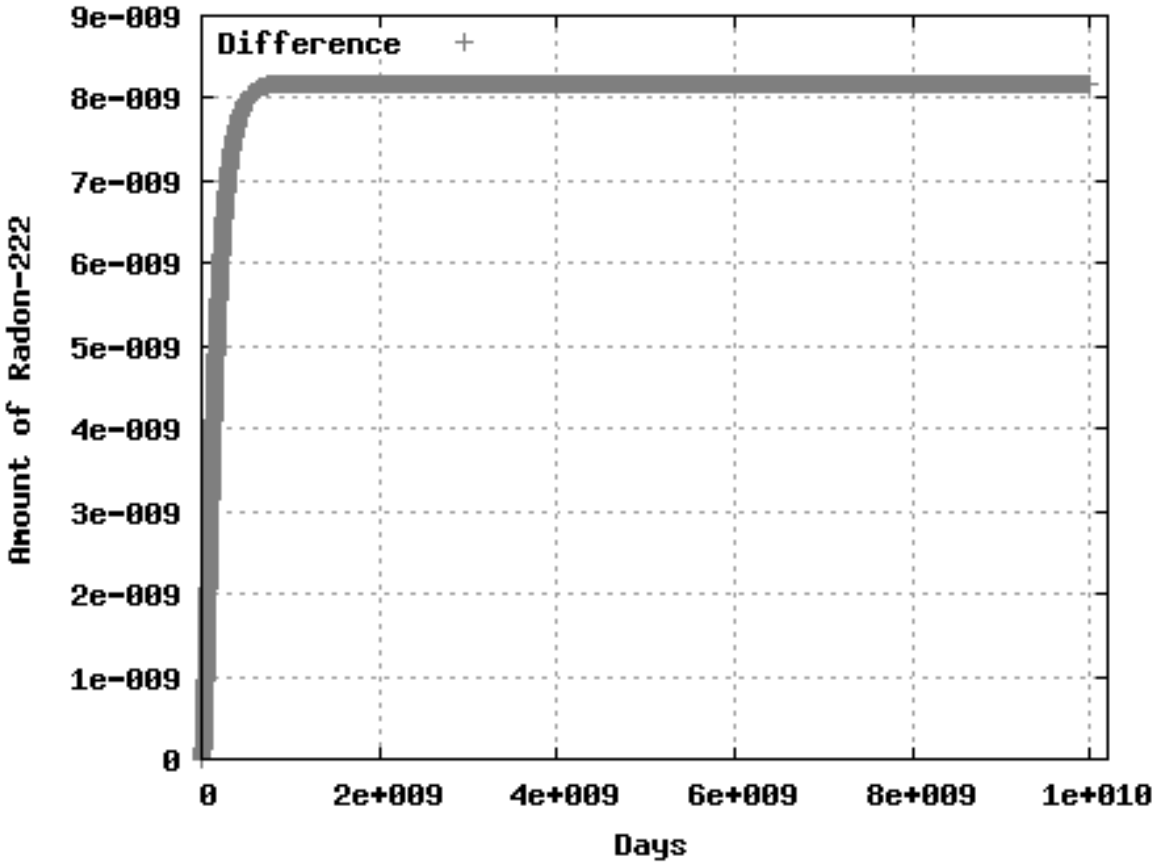
# Results

Numerical Solution for $^{222}Rn$ after $10^{10}$ days



# Results

Difference in the amount of $^{222}Rn$ in both cases after $10^{10}$ days.



# Conclusions

- Numerical results produced by Rosenbrock adaptive step method attend all the attributes of stability and consistence for a pre-defined precision for the natural decay chain of Uranium-238.
- The approach presented in this work for the natural decay chain of Uranium-238 guarantee s the convergence, consistency and stability of the numerical solution.
- Rosenbrock method can be used to solve problems involving the management of radioactive waste from the production of radioisotopes such as Technetium-99.
- For future work the idea is to study problems involving the management of radioactive waste from the production of radioisotopes.

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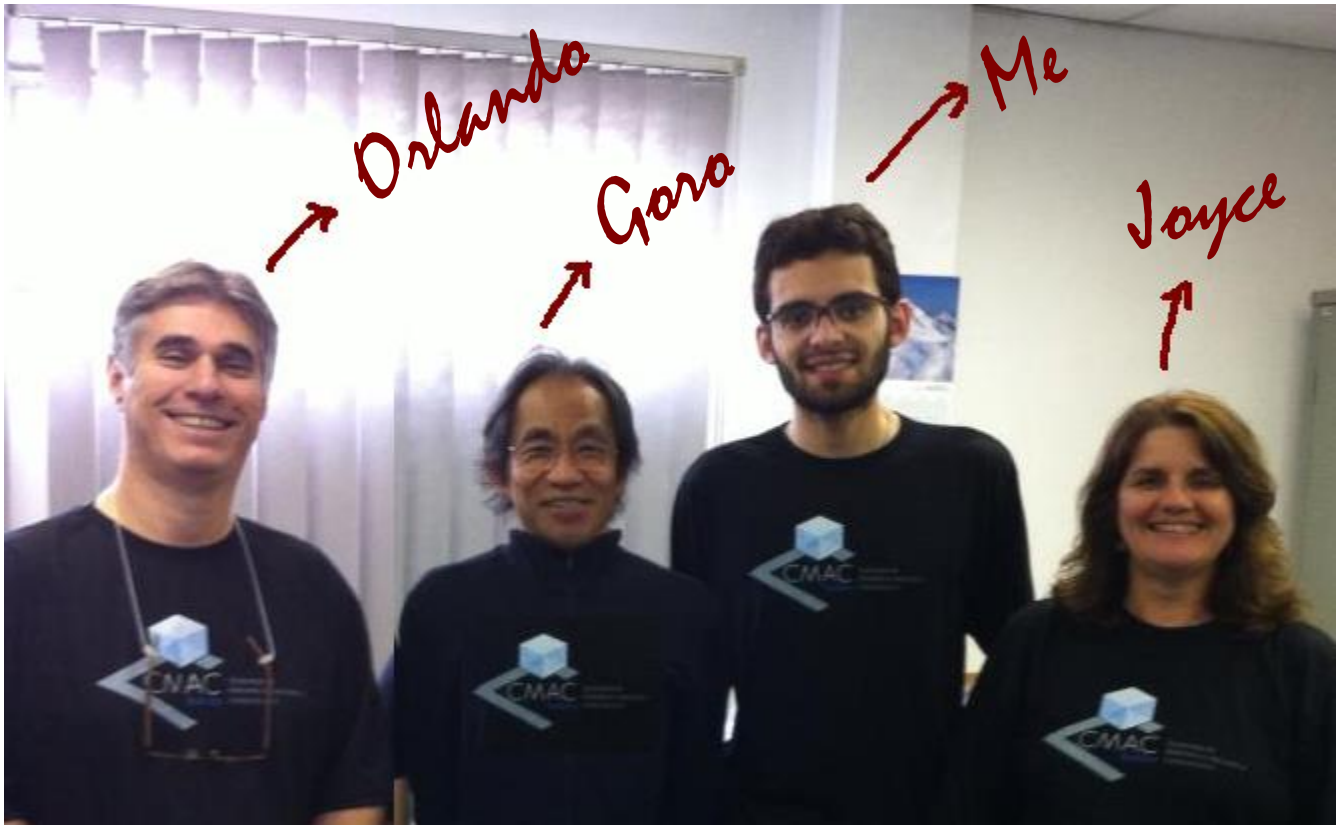
# Thanks!!!!!!

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