A hypothesis or theory is clear, decisive, and positive, but it is believed by no one but the person who created it. Experimental findings, on the other hand, are messy, inexact things, which are believed by everyone except the person who did that work.

> Harlow Shapley Through Rugged Ways to the Stars

University of Notre Dame

JINA Lecture Series on Tools and Toys in Nuclear Astrophysics

Nuclear Reaction Network Techniques

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Sites of the week

www.astrophysicsspectator.com/issues/issue2/issue2.13.html

www.unige.ch/~hairer/software.html

mathworld.wolfram.com/Jacobian.html

nobelprize.org/physics/laureates/1983/fowler-autobio.html

Syllabus

1 June 20 Purpose, Motivation, Forming a network, PP-chain code

2 June 21 Jacobian formation, Energy generation, Time integration, CNO-cycle code

3 June 22 Linear algebra, Thermodynamic trajectories, Alpha-chain code

4 June 23 Nuclear Statistical Equilibrium code, Big-Bang code

5 June 24 Networks in hydrodynamic simulations, General network code

Volume Constant

Jet.

Thermostat §

Y_A, Y_B, Y_C, Y_D, Y_E

 $A \leftarrow \frac{\alpha}{\beta} \rightarrow 2B$

3

 $A + C \leftarrow \frac{\gamma}{\delta} \rightarrow D$

 ε

And our reaction network takes the form

 $\dot{Y}_{A} = -\alpha Y_{A} + \beta Y_{B}^{2} - \gamma Y_{A}Y_{C} + \delta Y_{D} + \xi Y_{B}Y_{E}$

 $\dot{Y_{\rm B}} = 2\alpha Y_A - 2\beta Y_B^2 + \varepsilon Y_D - \xi Y_B Y_E$

 $\dot{Y}_{\rm C} = -\gamma Y_A Y_C + \delta Y_D + \xi Y_B Y_E$

 $\dot{Y}_{\rm D} = \gamma Y_A Y_C - \delta Y_D - \varepsilon Y_D$

 $\dot{Y}_{\rm E} = \varepsilon Y_D - \xi Y_B Y_E$

In terms of the reaction cross sections and molar abundances, this reaction network is described by the following set of ordinary differential equations

$$\dot{Y}_{i} = \sum_{j} C_{i} R_{j} Y_{j} + \sum_{jk} \frac{C_{i}}{C_{j}! C_{k}!} \rho N_{A} R_{jk} Y_{j} Y_{k} + \sum_{jkl} \frac{C_{i}}{C_{j}! C_{k}! C_{l}!} \rho^{2} N_{A}^{2} R_{jkl} Y_{j} Y_{k} Y_{l}$$



 $\dot{Y}_{\rm p} = -Y_{\rm p}Y_{\rm p}R_{\rm p,p} - Y_{\rm p}Y_{\rm d}R_{\rm p,d} + Y_{\rm 3he}Y_{\rm 3he}R_{\rm 3he,3he}$

 $\dot{Y}_{\rm d} = 0.5Y_{\rm p}Y_{\rm p}R_{\rm p,p} - Y_{\rm p}Y_{\rm d}R_{\rm p,d}$

 $Y_{3he} = Y_p Y_d R_{p,d} - Y_{he3} Y_{he3} R_{he3,he3}$

 $\dot{Y}_{4he} = 0.5 Y_{he3} Y_{he3} R_{he3,he3}$



Where the density and Avogadro number dependence has been folded into the reaction rates



The weights of the reactions are given for conditions in the Sun. The PP chains are the most important energy source in stars with masses less than 1.5 M_{sun} .

Abundance Variables

An atomic mass unit (amu) is defined as precisely 1/12 the mass of an atom of ¹²C at rest, unbound and in its ground state. The mass of an atomic mass unit is determined experimentally as 1.66053873x10⁻²⁴ g (2004 CODATA value).

Conceptually, an amu is equal to 1 gram divided by Avogadro's constant N_A. In imprecise terms, one amu is the average of the proton rest mass and the neutron rest mass. The mass of an atom in amu is roughly equal to the sum of the number of protons and neutrons in the nucleus.

Weak reaction terminology

 β^{-} decay : n \rightarrow p + e⁻ + $\overline{\nu_{e}}$ $(Z, A) \rightarrow (Z + 1, A) + e^{-} + \overline{\nu_{e}}$

 $\beta^+ \text{decay} : \mathbf{p} \to \mathbf{n} + \mathbf{e}^+ + \nu_{\mathbf{e}}$ $(Z, A) \to (Z - 1, A) + e^+ + \nu_e$

electron capture : $p + e^- \rightarrow n + \nu_e$ $(Z, A) + e^- \rightarrow (Z - 1, A) + \nu_e$

positron capture : $n + e^+ \rightarrow p + \overline{\nu_e}$ $(Z, A) + e^+ \rightarrow (Z + 1, A) + \overline{\nu_e}$

We may write our initial value problem as

$$\dot{Y}_{i} = \sum_{j} C_{i} R_{j} Y_{j} + \sum_{jk} \frac{C_{i}}{C_{j}! C_{k}!} \rho N_{A} R_{jk} Y_{j} Y_{k} + \sum_{jkl} \frac{C_{i}}{C_{j}! C_{k}! C_{l}!} \rho^{2} N_{A}^{2} R_{jkl} Y_{j} Y_{k} Y_{l}$$

or, in vector notation as

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$$

The ODE coefficients span orders of magnitude since the reaction rates depend on high powers of the temperature, and since the abundances themselves may traverse orders of magnitude. As a result, nuclear reaction networks are "stiff".

A rigorous definition is the ODEs are stiff if the negative, real part of the eigenvalues λ_j of the Jacobian matrix $\partial f/\partial y$ obey

 $S = \frac{\max |\operatorname{Re}(\lambda_j)|}{\min |\operatorname{Re}(\lambda_j)|} \gg 1$

 $S > 10^{15}$ is not uncommon in astrophysics.

Physically this means that some isotopes are changing on much faster timescales than other isotopes. PP-chain nucleosynthesis, which we examined yesterday and is responsible for most of the energy output of the Sun, offers an excellent example.

Practically speaking, stiffness means that an implicit time integration is generally needed to solve the initial value problem. This has two implications.

First, it means that an accurate Jacobian matrix ∂f/∂y must be available. Fortunately, the reaction network ODEs depend on simple powers of the composition variables, making the Jacobian easy to evaluate analytically.

Secondly, it means that we'll be solving (large) systems of linear equations. As the linear algebra will generally dominate the time to obtain a solution, we'll want to use efficient solvers.

It is interesting to examine the properties of a system containing only two species A and B coupled by forward and reverse reactions having rates R_A and R_B.

 $\frac{dY_A}{dt} = -Y_A R_A + Y_B R_B$ $\frac{dY_B}{dt} = Y_A R_A - Y_B R_B$

With the initial condition that $Y_B = 0$ at t = 0, this system has the analytic solution

$$\frac{Y_B}{Y_A} = \left[e^{(R_A + R_B)t} - 1\right] \left[\frac{R_B}{R_A}e^{(R_A + R_B)t} + 1\right]^{-1}$$

$$\frac{Y_B}{Y_A} = \left[e^{(R_A + R_B)t} - 1\right] \left[\frac{R_B}{R_A}e^{(R_A + R_B)t} + 1\right]^{-1}$$

Species A and B will approach their steady state equilibrium abundances, Y_B/Y_A= R_A/R_B, in a time roughly (R_A + R_B)⁻¹.

This means that equilibration between the pair occurs in a time determined by the most rapid rate coupling the two. This sometimes seems contrary to intuition.



$$\frac{Y_B}{Y_A} = \left[e^{(R_A + R_B)t} - 1\right] \left[\frac{R_B}{R_A}e^{(R_A + R_B)t} + 1\right]^{-1}$$

This solution illustrates the necessity of an implicit solution. When Y_A and Y_B have come into equilibrium one will want to take a large time step such that $R\Delta t \gg 1$.

If the ODEs are solved explicitly, the numerical oscillations will occur in the abundances, frequently leading to negative values.

 $Y_A^{t+1} = Y_A^t + \Delta t \left[-Y_A^t R_A + Y_B^t R_B \right]$ $Y_B^{t+1} = Y_B^t + \Delta t \left[Y_A^t R_A - Y_B^t R_B \right]$

If one evaluates the abundances on the right hand side of the ODEs at the new time, $Y_i + \partial Y_i$, and solves the resulting set of linear equations

$$\delta Y_A = -\delta Y_B = \frac{-Y_A R_A + Y_B R_B}{1/\Delta t + R_A + R_B}$$

The solution of the explicit solution, but for a large Δt the solution becomes insensitive to Δt and approaches the correct equilibrium solution.

• Consider the ${}^{12}C(\alpha,\gamma){}^{16}O$ reaction proceeding at a rate R.

 $\dot{Y}(^{4}\text{He}) = -Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$ $\dot{Y}(^{12}\text{C}) = -Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$ $\dot{Y}(^{16}\text{O}) = +Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$

Seach term on the right hand side contributes two Jacobian matrix elements:

$$J(^{4}\text{He},^{4}\text{He}) = \frac{\partial Y(^{4}\text{He})}{\partial Y(^{4}\text{He})} = -Y(^{12}\text{C}) R + \dots$$

 $J(^{4}\text{He},^{12}\text{C}) = \frac{\partial Y(^{4}\text{He})}{\partial Y(^{12}\text{C})} = -Y(^{4}\text{He}) R + \dots$

ODEs

 $\dot{Y}(^{4}\text{He}) = -Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$ $\dot{Y}(^{12}\text{C}) = -Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$ $\dot{Y}(^{16}\text{O}) = +Y(^{4}\text{He}) Y(^{12}\text{C}) R + \dots$

Jacobian elements $J(^{12}C, ^{4}He) = \frac{\partial Y(^{12}C)}{\partial Y(^{4}He)} = -Y(^{12}C) R + \dots$ $J(^{12}C,^{12}C) = \frac{\partial \dot{Y}(^{12}C)}{\partial Y(^{12}C)} = -Y(^{4}He) R + \dots$ $J({}^{16}\text{O}, {}^{4}\text{He}) = \frac{\partial \dot{Y}({}^{16}\text{O})}{\partial Y({}^{4}\text{He})} = +Y({}^{12}\text{C}) R + \dots$ $J({}^{16}\text{O}, {}^{12}\text{C}) = \frac{\partial \dot{Y}({}^{16}\text{O})}{\partial Y({}^{12}\text{C})} = +Y({}^{4}\text{He}) R + \dots$

The Jacobian matrix elements represent flows into (positive) or out of (negative) an isotope.

The matrices are not positive-definite or symmetric as the forward and reverse rates not usually equal, but they are typically diagonally dominant.



The pattern of nonzeros doesn't change with time, but each matrix element may change in magnitude and/or sign as the temperature, density, or abundances change with time.

The matrices are sparse, and get sparser as the number of isotopes increase.



In principal, every species reacts with every other species, resulting in a dense Jacobian matrix, but in practice it is possible to neglect most of these reactions.

Captures of free neutrons and isotopes of H and He on heavy nuclei occur much faster than fusions of heavier nuclei because of the Z_i Z_j dependence of the repulsive Coulomb term in the nuclear potential.



 Furthermore, with the exception of the PP-chains and Big Bang nucleosynthesis, reactions involving secondary isotopes of H (deuterium and tritium) and He are neglectable.

 Photodisintegrations also tend to eject free nucleons or α-particles.



Disintegration Christian Jehle, 2005

Thus, with a few important exceptions, for each nucleus we need only consider twelve reactions linking it to its nuclear neighbors by the capture of an n, p, α or γ and release a different one of these four.



Interlude



School of Athens 1510 Raffaello Sanzio

One of the most important consequences of changing the composition is the release (or absorption) of energy. The energy generation rate is given by

$$\dot{\epsilon}_{\rm nuc} = -\sum_{i} N_A M_i c^2 \dot{Y}_i - \dot{\epsilon}_{\nu} \quad (\text{erg g}^{-1} \text{ s}^{-1})$$

where M_ic^2 is the rest mass energy of species i.

The mass of a nucleus is conveniently expressed in terms of tabulations of the the atomic mass excess

 $M_i = A_i m_\mu + M_{\text{ex},i}$

where m_{μ} is the atomic mass unit.

The use of atomic mass units has the added benefit that electron conservation is correctly accounted for in the case of β⁻ decays and e⁻ captures, though reactions involving positrons require careful treatment.

The relationship between the binding energy of a nucleus and the mass excess is

$$E_{\text{bind},i} = Z_i M_{\text{ex},p} + N_i M_{\text{ex},n} - M_{\text{ex},i}$$

Thus, the nuclear energy generation rate may be written

$$\dot{\epsilon}_{\text{nuc}} = \sum_{i} N_A E_{\text{bind},i} \dot{Y}_i - \sum_{i} N_A (Z_i M_{\text{ex},p} + N_i M_{\text{ex},n}) \dot{Y}_i - \dot{\epsilon}_{\nu}$$

The energy lost to the freely streaming neutrinos has two components. One component comes from neutrino producing reactions and the other from thermal processes.



SN 1987a neutrino Irvine-Michigan-Brookhaven

Since neutrinos stream freely from the reaction site, this allows the simple replacement of the Mic² term in our previous expression with an averaged energy loss term.

$$\dot{\epsilon}_{\nu} = \sum_{i} \langle E_{\nu} \rangle \dot{Y}_{i,weak}$$

where we consider only those contributions to Ydot due to neutrino producing reactions.

Typically the average energy losses are performed by studying each nucleus individually, its excited state distribution, weak reaction strength distribution, etc. The results are then expressed as fitting functions, e.g., Langanke & Martinez-Pinedo, NucPhys A,673, 481 (2000)

Meutrino losses from thermal processes include

- Ø pair neutrino: e⁺ + e⁻ -> nu + nubar
- The photoneutrino: $e^- + \gamma > e^- + nu + nubar$
- Iasma neutrino: Yplasmon -> nu + nubar
- ø bremsstrahlung: e[−] + N(z,a) -> e[−] + N(z,a) + nu + nubar
- orecombination: e⁻ (continuum) -> e⁻ (bound) + nu + nubar

These calculations are difficult and the results are typically expressed in tables or fitting formulas. For example, Itoh et al. ApJS 102, 411, 1996 is used in the codes for these lectures.



A millimeter-wide pellet of hydrogen explodes under the multiple-angled fire of the Omega laser during a recent experiment at the Laboratory for Laser Energetics.

Given the initial conditions (constant temperature, constant density, starting composition), we wish to solve the stiff set of ODEs that represent our reaction network

 $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$

We'll take a look at several (but not all) methods of advancing the composition changes in time. Nearly all of these methods are in active use among various astrophysics researchers.

A good ODE integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize.

Sually the purpose of this adaptive stepsize control is to achieve some predetermined accuracy in the solution with minimum computational effort.

Many small steps should tiptoe through treacherous terrain, while a few great strides should speed through smooth uninteresting countryside.

The resulting gains in efficiency are not mere tens of percents or factors of two; they can sometimes be factors of ten, a hundred, or more.

Sometimes accuracy may be demanded not directly in the solution itself, but in some related conserved quantity that can be monitored.

Implementation of adaptive stepsize control requires that the stepping algorithm return information about its performance, most importantly, an estimate of its truncation error.

Obviously, the calculation of this information will add to the computational overhead, but the investment will generally be repaid handsomely.



 ${\it o}$ The simplest $1^{\rm rst}$ order Euler method moves the system $\dot{y}=f(y)$ over a time step h by

 $\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta$

where the change Δ is found by expanding $\mathbf{f}(\mathbf{y}_{n+1})$ about $\mathbf{f}(\mathbf{y}_n)$

 $(\tilde{\mathbf{1}}/h - \tilde{\mathbf{J}}) \cdot \Delta = \mathbf{f}(\mathbf{y}_n)$

which is simply

 $ilde{\mathbf{A}} \cdot \mathbf{x} = \mathbf{b}$

This method costs 1 Jacobian and 1 right-hand side evaluation,
 1 matrix reduction, and 1 backsubstitution.

This version of the Euler method has the smallest cost per time step and is one of the most common methods for evolving reaction networks.

The disadvantage is this method provides no rigorous estimate of the accuracy of the integration step.

Heuristics are invoked to gain some sense of accuracy and to form the next time step,. Such heuristics and are typically based upon limiting the change in any abundance, which is above some specified level (say 10⁻⁴ in mass fraction), to be less than some specified value (say, 5%).

This simplest 1^{rst} order Euler method can be improved somewhat by iterating on the basic time step formula

 $\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta$

that is, one seeks the zero of the function

 $z(\mathbf{y}) = \mathbf{y}_{n+1} - \mathbf{y}_n - \Delta = 0$

Iteration continues until the corrections are suitably small and the function is within some tolerance of zero. This provides the method with some measure of stability and convergence.

If this convergence does not occur within a reasonable number of iterations, the timestep is subdivided into smaller intervals until a converged solution can be achieved.

Mowever, a formal estimate of the truncation error is still not available (as it must be for any first order scheme).

The 1^{rst} Euler method could be modified to implement "step doubling" to gain a formal accuracy estimate; take two half step and one full step. If the two solutions agree within some specified accuracy tolerance, accept the time step.

Step doubling is expensive. Higher order methods obtain accuracy estimates by comparing solutions at different orders. We turn to two of these schemes next.

 ${\it @}$ The 4th order Kaps-Rentrop method advances a system $\dot{y}=f(y)$ over a time step h by

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \sum_{i=1}^{r} b_i \Delta_i$$

where the Δ_i are found from solving the staged equations

 $\tilde{\mathbf{A}} = (\tilde{\mathbf{1}}/\gamma h - \tilde{\mathbf{J}})$ $\tilde{\mathbf{A}} \cdot \Delta_1 = \mathbf{f}(\mathbf{y}_n)$

 $\tilde{\mathbf{A}} \cdot \Delta_2 = \mathbf{f}(\mathbf{y}_n + a_{21}\Delta_1) + c_{21}\Delta_1/h$

 $\tilde{\mathbf{A}} \cdot \Delta_3 = \mathbf{f}(\mathbf{y}_n + a_{31}\Delta_1 + a_{32}\Delta_2) + (c_{31}\Delta_1 + c_{32}\Delta_2)/h$ $\tilde{\mathbf{A}} \cdot \Delta_4 = \mathbf{f}(\mathbf{y}_n + a_{31}\Delta_1 + a_{32}\Delta_2) + (c_{41}\Delta_1 + c_{42}\Delta_2 + c_{43}\Delta_3)/h$

The bi, γ , a_{ij} , and c_{ij} are fixed constants of the method.

An estimate of the truncation error is made by comparing an embedded 3rd-order solution with the 4th-order solution. This in turn permits adaptive stepsize control.

 This method costs 1 Jacobian and 3 right-hand side evaluations, 1 matrix reduction, and 4 backsubstitutions for a time step that meets the specified integration accuracy.

Possessing an estimate of the integration accuracy seems well worth the small additional cost over the simplest Euler method; two extra evaluations of the right-hand side and three extra backsubstitutions.

The Note in this method not all of the right-hand sides are known in advance. (Δ_4 depends on Δ_3 ... depends on Δ_1).

This general feature of the higher-order integration methods examined in this lecture series will impact the optimal choice of a linear algebra package.



The variable order Bader-Deuflhard method advances a system $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ over a large time step H from \mathbf{y}_n to \mathbf{y}_{n+1} by forming h = H/m $\tilde{\mathbf{A}} = (\tilde{\mathbf{1}} - \tilde{\mathbf{J}})$ $\tilde{\mathbf{A}} \cdot \Delta_0 = h\mathbf{f}(\mathbf{y}_n)$ $\mathbf{y}_1 = \mathbf{y}_n + \Delta_0$

then for k=1,2 ... m-1 solving the staged equations $ilde{\mathbf{A}} \cdot \mathbf{x} = h\mathbf{f}(\mathbf{y}_k) - \Delta_{k-1}$ $\Delta_k = \Delta_{k-1} + 2\mathbf{x}$ $\mathbf{y}_{k+1} = \mathbf{y}_k + \Delta_k$

closure is obtained by the last stage

$$\mathbf{\hat{A}} \cdot \Delta_m = h[\mathbf{f}(\mathbf{y}_m) - \Delta_{m-1}]$$
$$\mathbf{y}_{n+1} = \mathbf{y}_m + \Delta_m$$

This staged sequence of matrix equations is executed at least twice with m=2 and m=6, which yields a 5th-order method.

The sequence may be executed a maximum of seven times, which yields a 15th-order method. The exact number of times the staged sequence is executed depends on the accuracy requirements and the smoothness of the solution.

Setimates of the accuracy of an integration step are made by comparing the solutions derived from different orders. This in turn permits adaptive stepsize control.

This method has a minimum cost of 1 Jacobian and 8 right-hand side evaluations, 2 matrix reductions, and 10 backsubstitutions for a time step that meets the specified integration accuracy.

The cost increases by 1 matrix reduction + m backsubstitutions for every order increase.

The cost per step is at least twice as large as the simple Euler or Kaps-Rentrop method, but it may be more efficient globally if accurate steps are at least twice as big can be taken.

The Bader-Deuflard method is used in the codes I'm providing for these JINA lectures.

Interlude



The Medical Alchemist Franz Christoph Janneck, (1703 – 1761) Oil on copper – 13" x 9"

It was independently suggested by Bethe & von Weizsäcker in 1939 that reactions of protons with carbon and nitrogen would provide competition with the PP-chains.

They showed that a series of reactions, called the CN cycle, had the property that CN nuclei served only as catalysts for the conversion of hydrogen into helium but were not themselves destroyed.



The basic CN cycle is

 ${}^{12}C(p,\gamma){}^{13}N(\beta^+\nu){}^{13}C$ ${}^{13}C(p,\gamma){}^{14}N$ ${}^{14}N(p,\gamma){}^{15}O(\beta^+\nu){}^{15}N$ ${}^{15}N(p,\alpha){}^{12}C$

Summing the particles before and after the cycle one obtains

 $^{12}C + 4H \rightarrow ^{12}C + ^{4}He + 2\beta^{+} + 2\nu$

the ¹²C nucleus only plays the role of a catalyst.

The same cycle occurs with any of the four nuclei ¹²C, ¹³C, ¹⁴N, ¹⁵N as catalyst, or any mixture of them.

In fact, a mixture of those nuclei must soon result regardless of the initial composition.

The energy generated is related to the reciprocal of the time it takes to go around the cycle multiplied by (4M_H - M_{He4})c² minus the energy loss in the two neutrinos.



It was later realized that all the stable oxygen isotopes provide additional cycles.



Prior to 1952 it was thought that the CNO cycles were mostly responsible for the energy generated in the sun.

However, Edwin Salpeter showed that the reaction rate of the proton chain was about an order of magnitude larger than previously believed.

This brought about a reversal in the roles thought to be played by the two hydrogen burning mechanisms in the Sun.



ican CAmerican Institute of Physics

We have implicitly assumed that the beta decay lifetimes were negligible. For 0.2 < T₉ < 0.5, the "hot" or "beta-limited" CNO cycles comes into play.



If $T_9 > 0.5$, then one breaks out of the beta-limited CNO cycles and begins a journey on the rapid-proton capture process.



Tasks for the day

Download, compile, and run the basic CNO cycle code from www.cococubed.com/code_pages/burn.shtml

Serify the ODEs and the Jacobian matrix elements CNO cycle 1.

Run the code for T = 30x10⁶ K, ρ = 100 g/cm³, and an initial composition of X(¹²C)=X(¹⁶O)=0.1. Plot the abundance evolution. What isotope is most abundant when the CNO cycle is in equilibrium? How long does it take for hydrogen to be depleted? Repeat for T = 300x10⁶ K. What do you conclude?

Repeat the problem above with the beta-limited CNO code.

Tasks for the day

Plot the pp-chain and CNO cycle energy generation rate as a function of temperature for a density suitable for the center of the Sun and solar metallically. What do you conclude about the relative contributions of each to the Sun?



Tools and Toys in Nuclear Astrophysics



Turns coal into diamonds