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A Short Introduction to Deterministic Calculations with ERANOS
Physical, Analytical and Numerical Basis of Deterministic Methods

Giacomo Grasso
Nuclear Engineering Laboratory of Montecuccolino
University of Bologna

Progettazione e Gestione di Sistemi Nucleari Avanzati
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Introducing ERANOS

ERANOS:

“European Reactor ANalysis Optimized System.”

ERANOS was developed by a joint effort of the main European nuclear research divisions in order to release the most advanced tool to be shared in Europe for the neutron design of nuclear reactors.

The result is a suite of modules inherited by the many contributions coming from all the existing European transport codes, together with a brand new cell code completing the environment.

The physical features have been also extended by adding brand new dynamic memory management techniques through the adoption of a suitably developed, low level programming language called “**esope**”.

The Human-Machine Interface (HMI) is represented by an input file listing all the operations to be processed for each execution of the code. The input file is formatted according to a syntax defined by a dedicated language, the “**Langage Utilisateur**” (“**LU**”). Besides the numerical techniques required to set up and run a simulation, the user can also introduce simple procedures for

- ▶ data management,
- ▶ system variables access,
- ▶ processed/processing data output,
- ▶ etc.

by simply querying the system in LU.

ERANOS Structure

The complex ERANOS environment is mainly based upon:

- ▶ basic data libraries;
- ▶ different methods and computational options defining a calculating scheme;
- ▶ integral experiences qualifying the methods;
- ▶ a validity domain.

ERANOS Calculating Schemes

The number of choices allowed in setting up a calculation let define two main schemes:

1. a **Reference Scheme**

where all the options have to be fixed to best suite the problem according to the reactor physics and the aimed precision;

2. a **Design Scheme**

where some simplifications are allowed with respect to the reference model - once the compromise in precision has been clearly pointed out - in order to be able to set up some repetitive calculations.

All the neutronic parameters of a reactor are obtained by weighting on the neutron flux, which describes the neutrons distribution in the core. The flux is the solution of the **Boltzmann equation**. The complexity of this equation requires **discrete and multigroups methods** for its numerical solution, summarized in two steps:

1. a number of **Cell Calculations**, and
2. the **Core Calculation** itself.

ERANOS - Basic Data Libraries

ERANOS needs to perform neutronic calculations based on the nuclear properties of the materials composing the problem. The main information sources for nuclear properties are the cross section data libraries, such as **ENDF/B**, **JEFF**, **JENDL**, etc.

ERANOS is distributed together with some proper libraries, suitably revised from the ENDF tapes to provide the cross section data in the form needed by the code. Every library distributed along with the code implements indeed:

- ▶ a **33 energy groups** (broad) cross section dataset for all the nuclides defined in the library;
- ▶ a **172 energy groups** cross section dataset for many (not all the) nuclides defined in the library, for a finer evaluation of the cross sections;
- ▶ a **175 energy groups** cross section dataset, mainly for damage or activation analyses, for all the nuclides defined in the library;
- ▶ a **1968 energy groups** (fine) cross section dataset for the most important nuclides included in the library, for the best evaluation of the cross sections.

ERANOS - Cell Calculations

In approaching a neutronic problem by deterministic methods, the most relevant question is the creation of specific data sets (cross sections vectors and both transport and scattering matrices) for the problem itself.

For every region defined in the simulation domain, a corresponding “cell” must be isolated and considered for local transport problems. Cells are therefore the elementary units describing the simulation domain.

The solution of the Boltzmann equation in each cell permits the retrieval of elementary information about the flux spectrum, by which the standard multigroup cross sections provided with the code libraries are weighted to obtain the effective multigroup cross sections for each region.

Within the ERANOS environment, the microscopic and macroscopic cross sections and matrices for use in reactor core calculations are provided by the **E**uropean **C**ell **C**ode (**ECCO**).

ERANOS - Reactor Calculations

The cell data can be organized in a complete model of the system for the reactor simulation. ERANOS can perform both diffusion or transport calculations to retrieve a complete set of information about the system:

- ▶ the critical mass;
- ▶ the reactivity worth of the fuel Burn Up (BU);
- ▶ the reactivity worth of the Control Rods (CRs);
- ▶ the reactivity worth of the operating conditions;
- ▶ the Doppler effect;
- ▶ the effect of a partial or complete coolant voiding;
- ▶ the spatial distributions of:
 - ▶ the linear and volumetric power,
 - ▶ the flux,
 - ▶ the structural damaging.

The Boltzmann Equation I

The distribution of neutrons in a medium is governed by the Boltzmann equation, representing a net balance for the neutrons population in a generic infinitesimal volume of the 6-dimensional phase space.

The integro-differential form of the time-independent Boltzmann equation, depending on the angular neutrons flux $\Psi(\vec{r}, E, \hat{\Omega})$ is, from the reactor physics:

$$\begin{aligned} \hat{\Omega} \cdot \nabla \Psi(\vec{r}, E, \hat{\Omega}) + \Sigma_t(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}) = \\ = \int \int \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \Psi(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}' + S(\vec{r}, E, \hat{\Omega}). \end{aligned} \quad (1)$$

Among the various terms of the neutrons balance, it is worth noticing:

- ▶ a **diffusion term** for balancing the population upon the neutrons streaming through the infinitesimal volume;
- ▶ a **collisional term** for taking into account all the neutrons abandoning the phase space volume as a consequence of a generic collision event (scattering to other energies or removal);
- ▶ a **scattering source term** to consider the neutrons incoming in the infinitesimal volume from the rest of the phase space after a scattering collision;

The Boltzmann Equation II

The same equation can be expressed in integral form, thus eliminating the explicit dependence upon the flight direction $\hat{\Omega}$. The balance equation refers now to the scalar neutrons flux $\Phi(\vec{r}, E)$ by:

$$\Phi(\vec{r}, E) = \int \left\{ \int \Sigma_s(\vec{r}', E' \rightarrow E) \Phi(\vec{r}', E') dE' + S(\vec{r}', E) \right\} \frac{e^{-\Sigma_t |\vec{r}' - \vec{r}|}}{4\pi |\vec{r}' - \vec{r}|^2} d\vec{r}' . \quad (2)$$

The equivalence of the two formulations can be understood by noticing that the outermost integral is extended over the whole space to search for contributions to the population in the considered phase space volume. The transport contribution to the balance is implicitly introduced in the source terms by means of the probability of non collision in the $\vec{r}' - \vec{r}$ path:

$$e^{-\Sigma_t |\vec{r}' - \vec{r}|} .$$

The Fission Source for Multiplying Media

The source term, either $S(\vec{r}, E, \hat{\Omega})$ or $S(\vec{r}, E)$, for a multiplying medium, contains a fission contribution given by

$$S_f(\vec{r}, E, \hat{\Omega}) = \frac{1}{4\pi} \iint \chi(E, E') \bar{\nu}(E') \Sigma_f(E') \Psi(\vec{r}, E', \hat{\Omega}') dE' d\hat{\Omega}'$$

for the integro-differential Boltzmann equation (1). For the integral formulation of the same equation (2), the same contribution can be written as

$$S_f(\vec{r}, E) = \int \chi(E, E') \bar{\nu}(E') \Sigma_f(E') \Phi(\vec{r}, E') dE'.$$

In both formulations, the term $\chi(E, E')$ represents the energy dependent fission spectrum, while the $\bar{\nu}(E')$ term is the energy dependent, mean number of secondary neutrons released by fission.

Monte Carlo vs Deterministic Method I

Method Monte Carlo methods obtain answers by simulating individual particles and recording some aspects of their average behavior. The average behavior of particles in the physical system is then inferred (using the **Central Limit Theorem**) from the average behavior of the simulated particles. By contrast, deterministic methods (the most common of which is the discrete ordinates method) analytically solve approximated formulations of the transport equation to retrieve the average particle behavior.

Solution Whilst Monte Carlo methods supply information only about specific requests by the user, deterministic methods typically give fairly complete information (for example, flux) throughout the phase space of the problem.

Monte Carlo vs Deterministic Method II

Monte Carlo methods transport particles between events (for example, collisions) that are separated in space and time. Neither differential space nor time are inherent parameters of Monte Carlo transport. The integral equation does not have terms involving time or space derivatives.

By contrast, the discrete ordinates method visualizes the phase space to be divided into many small boxes, and the particles move from one box to another. In the limit, as the boxes get progressively smaller, particles moving from box to box take a differential amount of time to move a differential distance in space. In the limit, this approaches the integro-differential transport equation, which has derivatives in space and time.

Solution Methods

The Boltzmann equation is too complicated to retrieve analytical solutions but for very simplified models. To approach actual problems, many techniques have been developed for an approximated solution of either equation (1) or (2).

All the approximated solution techniques can be classified into three categories:

1. analytic-numerical methods for the integro-differential equation approximation (i.e.: P_N , B_N and S_N methods);
2. numerical methods for the solution of the integral equation (i.e.: the numerical approximation of the collision probability integrals);
3. diffusion approximation.

Multigroup Approximation

The preliminary hypothesis common to all the methods is represented by the discretization of the problem with respect to the continuous energy variable: its domain is thus segmented into N_g intervals called “groups”.

Since all the parameters of either equation (1) or (2) explicitly depend on energy, in order to apply the discretization a set of N_g values has to be pointed out for every parameter, being representative of the continuous behavior of the parameter within each energetic group. The definition of these multigroup constants is performed by integrating the value of each parameter in every group by weighting on the flux, according to

$$A_g = \frac{\int_{\Delta E_g} A(E)\Phi(E)dE}{\int_{\Delta E_g} \Phi(E)dE} \quad g = 1, \dots, N_g. \quad (3)$$

Under such hypothesis, the Boltzmann equation reduces to a set of N_g equations in the Φ_g unknowns (each one defined as the denominator of the corresponding equation (3)).

Multigroup Approximation for Homogeneous Media

For a homogeneous medium, the spatial behavior of both the flux and the source can be assumed in a fundamental mode defined by the **Buckling B** of the system:

$$\Psi(\vec{r}, E, \hat{\Omega}) = \Psi(E, \hat{\Omega}) e^{i\vec{B} \cdot \vec{r}}, \quad (4)$$

so that the multigroup formulation of equation (1) becomes

$$(i\vec{B} \cdot \hat{\Omega} + \Sigma_{t,g})\Psi_g(\hat{\Omega}) = \int \Sigma_{s,g'}(g' \rightarrow g, \hat{\Omega}' \rightarrow \hat{\Omega})\Psi_{g'}(\hat{\Omega}')d\hat{\Omega}' + S_g(\hat{\Omega}). \quad (5)$$

The Spherical Harmonics Expansion I

Each equation of (5), integral in $\hat{\Omega}$, can be solved by expanding into spherical harmonics (Legendre polynomials) the flux and the scattering matrix:

$$2\pi\Psi_g(\hat{\Omega}) = \Psi_g(\mu) = \sum_{l=0,\dots,\infty} \frac{2l+1}{2} \Psi_{l,g} P_l(\mu)$$

$$\Sigma_s(g' \rightarrow g, \mu) = \sum_{l=0,\dots,\infty} \frac{2l+1}{2} \Sigma_{s,l}(g' \rightarrow g) P_l(\mu).$$

The P_l polynomials can be seen as bi-dimensional, elementary distribution “modes” making up an orthonormal basis for the space of angular distributions. By this assumption, the Ψ_l and $\Sigma_{s,l}$ coefficients of the two expansions represent the weights of each “mode” composing the actual distributions.

Another way to think about the spherical harmonics expansion is the frequency processing of a signal. Each wave can be always represented as a composition of elementary waves, each one defined by its elementary frequency. The coefficients of the decomposition represent the relative importances of the different contributions to the original signal.

The Spherical Harmonics Expansion II

The equation for a single component of the flux can be extracted from the expansion in series of Legendre polynomials by simply projecting the latter on a single harmonic m (multiplying thus by the corresponding harmonic P_m and integrating over all μ). The resulting system for the infinite components of the flux is:

$$(m+1)\iota B \Psi_{m+1,g} + m \iota B \Psi_{m-1,g} + \Sigma_t \Psi_{m,g} = \sum_{g'} \Sigma_{s,m}(g' \rightarrow g) \Psi_{m,g} + S_g. \quad (6)$$

It is worth noticing that the $\iota \vec{B} \cdot \hat{\Omega} \Psi_g(\hat{\Omega})$ term introduces, in the equation for a generic moment m , a dependence upon the adjacent $(m \pm 1)$ moments¹. This mutual dependence makes impossible to close a system of whatever number m of moments, being always necessary to include the $m+1$ moment too, and so on. Nonetheless, no approximation has been introduced in the present treatment as far as the whole, infinite system is concerned.

On the other side, there's clearly no way to treat a system of infinite equations, thus suitable approximations are needed to define proper criteria for the truncation of the system.

¹The expansion of the $\hat{\Omega} \Psi_g(\hat{\Omega})$ term leads to a number of contributions $(2l+1)\mu P_l(\mu)$ which, by means of the recurrence formula (see Appendices for details), equal $(l+1)P_{l+1}(\mu) + lP_{l-1}(\mu)$.

The P_N Method I

The P_N approximation is based on the assumption that $\Psi_{N+1} = 0$: the system can therefore be closed, becoming

$$\imath B \Psi_{1,g} + \Sigma_{t,g} \Psi_{0,g} = \sum_{g'} \Sigma_{s,0}(g' \rightarrow g) \Psi_{0,g} + S_g \quad (7)$$

$$\frac{\imath B}{3} \Psi_{0,g} + A_{1,g}(B, N) \Psi_{1,g} = \sum_{g'} \Sigma_{s,1}(g' \rightarrow g) \Psi_{1,g} \quad (8)$$

$$\Psi_{l,g} = -\frac{l}{2l+1} \imath B \frac{\Psi_{l+1,g}}{A_{l,g}(B, N)} \quad l = 2, \dots, N. \quad (9)$$

The P_N Method II

The $A_{l,g}(B, N)$ coefficients are expressed as a continuous fraction as

$$A_{l,g}(B, N) = b_{l-1} + \left(\frac{a_l}{b_l} + \left(\frac{a_{l+1}}{b_{l+1}} + \cdots + \frac{a_{N-1}}{b_{N-1}} \right) \right)$$

$$a_l = B^2 \frac{(l+1)^2}{(2l+1)(2l+3)}$$

$$b_0 = \Sigma_{t,g}$$

$$b_l = \Sigma_{t,g} - \sum_{g' \neq g} \Sigma_{s,l+1}(g \rightarrow g').$$

The B_N Method

The same expansion in spherical harmonics is performed in the B_N method, but the equation to be projected is divided in advance by $(\imath B\mu + \Sigma_t)$.

The infinite hierarchy of moment equations is truncated by assuming the N -th anisotropy order of the scattering source equal 0:

$$\Sigma_{s,l}(g' \rightarrow g)\Psi_{l,g} = 0 \quad \forall l \geq N,$$

thus obtaining a system equivalent to (7), with A_l coefficients parallel to those of the P_N method but for the b_l coefficients form, given by

$$b_0 = \begin{cases} \frac{B \operatorname{arctg}\left(\frac{B}{\Sigma}\right)}{3\left(1 - \left(\frac{\Sigma}{B}\right) \operatorname{arctg}\left(\frac{B}{\Sigma}\right)\right)} & \text{for } N = 1 \\ \Sigma_t B & \text{for } N > 1 \end{cases}$$

$$b_1 = \Sigma_{t,g} - \sum_{g' \neq g} \Sigma_{s,l+1}(g \rightarrow g')$$

$$b_{N-1} = \Sigma_{t,g} - \sum_{g' \neq g} \Sigma_{s,N}(g \rightarrow g') + \imath B \frac{N+1}{2N+1} \frac{-Q_{N+1} \frac{\Sigma}{\imath B}}{-Q_N \frac{\Sigma}{\imath B}}.$$

Consistent and Inconsistent P_1/B_1 Solutions I

By truncating the P_N or B_N expansions to the first moment, the two equations reduced system

$$iB J_g + \Sigma_r \Phi_g = S_{g,0} + \sum_{g' \neq g} \Sigma_{s,0}(g' \rightarrow g) \Phi_{g'} \quad (10)$$

$$-\frac{iB}{3} \Phi_g + \gamma \Sigma_{t,1} J_g = S_{g,1} + \sum_{g' \neq g} \Sigma_{s,1}(g' \rightarrow g) J_{g'} + \Sigma_{s,1}(g \rightarrow g) J_g, \quad (11)$$

where

$$\gamma = \begin{Bmatrix} 1 & P_1 \\ \frac{b_0}{\Sigma_{t,1}} & B_1 \end{Bmatrix},$$

leads to the s.c. **consistent solution** in both the 0-th order moment, Φ (the **scalar flux**), and the first one $\vec{J}$ (the **current**).

Consistent and Inconsistent P_1/B_1 Solutions II

The computation of the coefficients can be simplified by introducing the s.c. **extended transport approximation**, consisting of assuming

$$\sum_{g'} \Sigma_{s,1}(g' \rightarrow g) J_{g'} = \Sigma_{s,1}(g) J_g. \quad (12)$$

Under such hypothesis, the system (10) can be further simplified in the

$$\imath B J_g + \Sigma_r \Phi_g = S_{g,0} + \sum_{g' \neq g} \Sigma_{s,0}(g' \rightarrow g) \Phi_{g'} \quad (13)$$

$$-\frac{\imath B}{3} \Phi_g + \gamma \Sigma_{t,1} J_g = S_{g,1} + \Sigma_{s,1}(g) J_g, \quad (14)$$

leading to the s.c. **inconsistent solution**.

The Diffusion Equation

From the P_1 system, under the hypothesis of extended transport approximation, (13), in the fundamental mode ($\nabla = i\vec{B}$), the second equation assumes the form

$$\vec{J} = -\frac{1}{3(\Sigma_t - \Sigma_{s,1})} \frac{\partial \Phi}{\partial \vec{r}}.$$

Defined now:

$$\begin{aligned} \langle \mu \rangle &= \frac{\Sigma_{s,1}}{\Sigma_{s,0}} \text{ as the averaged cosine of the scattering angle,} \\ \Sigma_{tr} &= \Sigma_{t,0} - \langle \mu \rangle \Sigma_{s,0} \text{ as the transport cross section, and} \\ D &= \frac{1}{3\Sigma_{tr}} \text{ as the diffusion coefficient,} \end{aligned}$$

the latter equation assumes the well known **Fick law** form:

$$\vec{J} = -D \frac{\partial \Phi}{\partial \vec{r}}. \quad (15)$$

The first equation of (13) becomes then the **Diffusion Equation**:

$$\Sigma_r \Phi_g - \nabla(D \nabla \Phi_g) = S_{g,0} + \sum_{g' \neq g} \Sigma_{s,0}(g' \rightarrow g) \Phi_{g'}. \quad (16)$$

The S_N Method

The **Discrete Ordinate Method** is based on the segmentation of the solid angle into N discrete directions, projecting into these the angular flux by integrating the $\hat{\Omega}$ variable.

An approximation is introduced, assuming a linear dependence of the angular flux within each angular bin.

The Boltzmann equation thus assumes the form

$$\hat{\Omega} \cdot \frac{\partial \Psi}{\partial \vec{r}} + DB^2 \Psi + \Sigma_t \Psi = S. \quad (17)$$

The Collision Probabilities Method I

The main approach for solving the Boltzmann equation in heterogeneous media is based on the decomposition of the domain into N elementary and separate regions, for each of whom the neutronic parameters can be assumed constant.

The spatial integration of equation (2) in each region leads to a set of N equations like

$$V_i \Sigma_{t,i} \Phi_i = \sum_j P_{ij} V_j (\Sigma_{s,j} \Phi_j + S_j), \quad (18)$$

where

$$\begin{aligned} \Phi_j &= \frac{1}{V_j} \int_{V_j} \Phi(\vec{r}) d\vec{r} \\ S_j &= \frac{1}{V_j} \int_{V_j} S(\vec{r}) d\vec{r} \\ P_{ij} &= \frac{\int_{V_j} \Sigma_t(\vec{r}') \int_{V_i} (\Sigma_s \Phi(\vec{r}) + S(\vec{r})) \frac{e^{-\Sigma_t S}}{4\pi S^2} d\vec{r}' d\vec{r}}{\int_{V_i} (\Sigma_s \Phi(\vec{r}) + S(\vec{r}))}. \end{aligned}$$

The Collision Probabilities Method II

The P_{ij} terms represent the **Collision Probabilities**, i.e. the probabilities for a neutron produced in the i -th region to first collide in the j -th cell. Whether the regions are sufficiently small, the neutrons source can be considered punctual, thus reducing the collision probability to the form

$$P_{ij} \approx \frac{\Sigma_{t,j}}{V_i} \int_{V_j} \int_{V_i} \frac{e^{-\Sigma_t S}}{4\pi S^2} d\vec{r}' d\vec{r}.$$

According to the Collision Probabilities method, the solution of the Boltzmann integral equation is performed in two steps:

- ▶ computation of the collision probabilities P_{ij} and
- ▶ computation of the fluxes by means of the (18).

The complexity of the method is condensed in the first step, with the solution of N^2 double integrals for the computation of the collision probabilities. The latter are collected to build up a connection matrix for the definition of a system of linear equations in the fluxes (step two).

The Finite Difference Method I

Whatever method chosen to approximate the Boltzmann equation, the spatial dependence of the variables must be made explicit by discretizing the continuous domain. A simulation grid is therefore superposed to the actual domain, on each point of which both the variables and the unknowns are defined and computed.

Each equation resulting from the approximated method is then splitted in a set of punctual equations. The presence of the derivative operators introduces mutual dependences of the unknowns defined on neighboring nodes.

The derivative operator can be discretized by following its elementary definition as limit of the incremental ratio (e.g.: the derivatives of the flux about the i -th node, along the x direction):

$$\begin{aligned}\frac{\partial \Phi_i}{\partial x} &= \frac{\Phi_{i+1} - \Phi_{i-1}}{2\Delta x} \\ \frac{\partial^2 \Phi_i}{\partial x^2} &= \frac{\Phi_{i+1} - 2\Phi_i + \Phi_{i-1}}{\Delta x^2} .\end{aligned}$$

The Finite Difference Method II

Once the computational mesh is defined, a node labeling (e.g.: numbering) must be introduced to univocally associate each unknown to the proper node.

The most common node labeling scheme is based on the progressive numbering of the nodes by scanning progressively each direction, fixed the other ones.

Example

In a three dimensional problem, once the three directions have been discretized in N_x , N_y and N_z nodes respectively, and following the x-y-z order, the generic node (i, j, k) where $1 \leq i \leq N_x$, $1 \leq j \leq N_y$ and $1 \leq k \leq N_z$, is labeled

$$n = (k - 1) \cdot N_x \cdot N_y + (j - 1) \cdot N_x + i.$$

The Finite Difference Method III

The set of punctual equations, together with the appropriate boundary conditions, defines a matrix problem

$$\underline{A}\vec{\Phi} = \vec{b}, \quad (19)$$

since each equation for the unknown Φ_i depends on the unknowns Φ_j of the neighboring nodes j according to the s.c. “diamond” scheme²: the flux on each node depends on the flux at both the preceding and following node, in each direction.

According to this, and assuming the natural node labeling, the matrix $\underline{A}$ assumes a diagonal form (the number of non-zero diagonals being univocally defined by the dimensionality of the domain: 3, 5 and 7 diagonals for a 1D, 2D and 3D problem, respectively).

²The diamond scheme follows from the form of the operators involved in the problem, i.e. the Laplacian, the absorption, the scattering and the multiplicative operators.

Linear System Solution

Although the formal solution of eq. (19) is extremely easy, i.e.

$$\vec{\Phi} = \underline{A}^{-1} \vec{b} ,$$

the numerical inversion of such a huge (and sparse) matrix may result a very hard (and unfavorable) task. Several methods, both direct and iterative, have been developed then in order to get the solution in a cheaper but equivalent way.

The Gauss Method I

Direct methods for the solution of linear equations systems are based on the analytical solution of the problem, approached in a numerical way.

The most common direct method for the solution of a linear equations system is the Gauss one. It is based on the triangularization of the coefficient matrix $\underline{A}$ by a univocal succession of operations by row (pivoting procedure). The sequence of operations can be formalized by a unique matrix operator $\underline{S}$ (see appendices for details). At least, by applying the same succession of operations to the right hand side (rhs) vector $\vec{b}$ too, the equivalence of the transformed equation with respect to the original one is guaranteed. Formally, the new problem becomes then

$$\underline{\tilde{A}}\vec{\Phi} = \vec{\tilde{b}},$$

where $\underline{\tilde{A}}$ and $\vec{\tilde{b}}$ have been obtained according to the transformation

$$\begin{aligned}\mathcal{T} : \vec{x} &\longrightarrow \vec{\tilde{x}} \\ \vec{\tilde{x}} &= \underline{S}\vec{x}.\end{aligned}$$

The Gauss Method II

The upper-triangular form of the transformed coefficient matrix $\tilde{A}$ permits an analytical approach to the problem, by solving the set of equations in **reverse cascade order**.

The last equation results indeed independent on the remaining ones, being the dependences on the “neighboring” unknowns incorporated into the remaining equations by the pivoting procedure. Once the last equation has been solved, by proceeding in reverse order the solution of the remaining equations immediately follows, since the dependence of the relative unknowns on already computed values of the flux only.

Iterative Solution Methods

Iterative methods for the solution of linear equations systems are based on the successive refinement of trial solutions imposed to the system.

Since the mutual dependence of the unknowns, a trial value to one/a set of them reflects in a modification of all the remaining. A feedback information is then sent to the starting unknown/set, and the process iterated. Many methods have been developed then, aiming at an optimization of the feedback process by accelerating the propagation of the informations through the grid (strictly dependent on the coefficient matrix form).

The dependence of iterative methods upon the initial trial solution is a main drawback of such methods. This numerical dependence is condensed into the coefficient matrix only, thus is an intrinsic property of the physical problem to be solved. Matricial problems can be then classified into **well** and **bad defined**: the former being all those problems for which the solution error is reduced at every solution step, *vice versa* the latter (see appendices for further informations).

Every iterative method intrinsically requires a convergence criterion to establish, after each step, whether the solution has been reached or not. The convergence criterion is often chosen as the precision of the numerical solution.

Iterative vs Direct Methods

The main differences between iterative and direct solution methods are the precision of the computed solution and the computation time needed to retrieve the latter:

- ▶ Direct methods are analytically exact by definition; on the other side, iterative methods are all based upon successive refinements of a trial solution.
- ▶ Direct methods solve the matrix problem in a single step, during which a huge number of operations is performed. Iterative methods are based instead on many steps procedures, a small number of operations being performed at each step.

In order to “compare” these differences, it is to be taken into account that as far as the required precision of an iterative method increases, the computational time quickly rises up to order of magnitude proper of direct methods. On the other side, the numerical errors intrinsic in every numeric algorithm act in limiting both the theoretical “charm” of direct methods and the maximum precision demandable to iterative methods.

The choice of one method rather than another one thus depends only on the compromise between precision and performances the user intends to accept.

The Jacobi Method

The basic idea of the Jacobi Method is the decoupling of the solution at each step from the solution at the previous one. Based on each temporary solution, the new one is calculated upon the latter, assumed as constant.

Formally the problem is written by splitting the coefficient matrix into its diagonal and non-diagonal parts:

$$\underline{A} = \underline{D} - \underline{C}.$$

Starting from this, the matrix problem is written as

$$\underline{D}\vec{\Phi} = \underline{C}\vec{\Phi} + \vec{b}.$$

No simplifications nor approximations have been introduced by now.

Starting from this, the solution of the problem at step ℓ , $\vec{\Phi}^{(\ell)}$, is computed by decoupling it from the solution at step $\ell - 1$, which is assumed as a known term. Thus the rhs of the previous equation is considered completely known, and the system easily solved. The formal expression of the Jacobi method is therefore

$$\underline{D}\vec{\Phi}^{(\ell)} = \underline{C}\vec{\Phi}^{(\ell-1)} + \vec{b}. \quad (20)$$

The Gauss-Seidel Method

An evolution of the Jacobi method is represented by the Gauss-Seidel method. The basic idea is that the convergence of iterative methods strongly depends on the speed of propagation of information through the grid. According to the method of Jacobi, the informations obtained at each step cannot be used but in the following one. Since the solution of the equations of the matrix problem is sequential, the Gauss-Seidel method foresees the use of all the information already collected in the present step to compute the remaining unknowns. This idea permits to accelerate the propagation of “fresh” information immediately after it is retrieved rather than after a whole step.

To formalize this, it is necessary to split the non-diagonal part of the coefficient matrix into its upper $\underline{U}$ and lower $\underline{L}$ parts. Equation (20) then becomes

$$\underline{D}\vec{\Phi}^{(\ell)} = \underline{U}\vec{\Phi}^{(\ell)} + \underline{L}\vec{\Phi}^{(\ell-1)} + \vec{b}. \quad (21)$$

The SOR Method I

Proposed by the American mathematician Young in 1950, the Successive Over Relaxations method applies a correction to the Gauss-Seidel one aiming at dumping the solution oscillations around the “true” value during iterations.

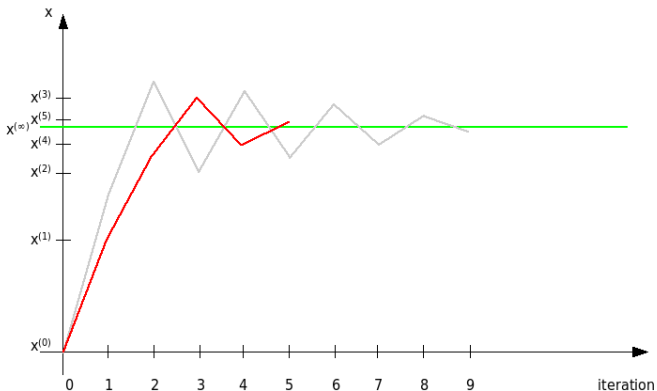
As shown in appendix, applying the coefficient matrix to a different vector than the solution, causes the new temporary estimate to be whatever generic vector but the solution. If the matrix problem is well posed, it is known also that the distance in norm of the temporary solutions decreases along the iterations: this causes the temporary solution to oscillate around the “true” value.

The key point of the SOR method is the computing of the new estimate of the solution $\vec{\Phi}_{\text{SOR}}^{(\ell)}$, as a weighted contribution of both the Gauss-Seidel evaluation $\vec{\Phi}_{\text{G-S}}^{(\ell)}$ and the precedent estimate $\vec{\Phi}^{(\ell-1)}$: since the latter two contributions lie on different hemispaces, with respect to the “true” solution, a properly weighted mean would result in a net speed up of convergence.

$$\vec{\Phi}^{(\ell)} = \omega \underline{D}^{-1} \left(\underline{U} \vec{\Phi}^{(\ell)} + \underline{L} \vec{\Phi}^{(\ell-1)} + \vec{b} \right) + (1 - \omega) \vec{\Phi}^{(\ell-1)}. \quad (22)$$

The SOR Method II

A graphical Representation of the SOR weighting between old and expected solutions is presented in figure.



The SOR Method III

The effectiveness of the SOR method strongly depends upon the choice of the overrelaxation parameter ω . The convergence itself of the method is guaranteed by the necessary condition $0 < \omega < 2$, which is also sufficient if the coefficient matrix $\underline{A}$ is diagonally dominant.

Noticing that, for $\omega = 1$ the SOR method reduces to the Gauss-Seidel one, it can be shown that, for different choices of the overrelaxation parameter, the SOR method can be also used to solve diverging problems.

The optimal choice of the overrelaxation parameter, for convergence speed up aims, must strictly depend on the coefficient matrix $\underline{A}$. At each step, both the spread and centering of the gap between the old and the new Gauss-Seidel solutions depend on the coefficient matrix applied to the former evaluate to retrieve the latter one: the overrelaxation parameter should therefore depend on the iteration operator (i.e.: the coefficient matrix) to let the weighted mean coincide with the “true” solution. It can be shown that the optimal value for the overrelaxation parameter is related to the spectral radius of matrix $\underline{A}$ as

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho_{\underline{A}}^2}} .$$

Summary

ERANOS is a powerful suite of deterministic codes for the solution of the Boltzmann equation in multiplying systems.

The ERANOS environment collects the state-of-the-art of the European methods for both cell and reactor calculations.

The main approximation methods for transport and diffusion calculations of actual geometries are included in the suite.

The code implements also the methods for the numerical discretization of the approximated transport equation, together with many techniques for accelerating the convergence of the solution.

APPENDIXES

The Legendre Polynomials I

The Legendre Polynomials, expressed using the Rodrigues' formula as

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} [(x^2 - 1)^l] \quad (23)$$

are l -th degree orthogonal polynomials resulting from the solution of the Legendre equation

$$\frac{d}{dx} \left[(1 - x^2) \frac{d}{dx} P_l(x) \right] + l(l+1) P_l(x) = 0.$$

for integer $l = 0, 1, 2, \dots$ and with the normalization $P_l(1) = 1$.

It can be seen indeed that the Legendre equation has regular singular points at $x = \pm 1$ so, in general, a series solution about the origin will only converge for $|x| < 1$. When n is an integer, the solution $P_l(x)$ that is regular at $x = 1$ is also regular at $x = -1$, and the series for this solution terminates, i.e. is a polynomial.

The Legendre Polynomials II

Two important properties of Legendre Polynomials are:

- ▶ their orthogonality with respect to a scalar product defined by integrating the product of two different polynomials over the whole domain $[-1, 1]$:

$$\int_{-1}^1 P_l(x)P_m(x)dx = \frac{2\delta_{lm}}{2l+1},$$

where δ_{lm} is the Kronecker delta;

- ▶ the formula of recursion, given as

$$(2l+1)P_l(x) = (l+1)P_{l+1}(x) + lP_{l-1}(x).$$

The Associated Legendre Functions

The Associated Legendre Functions, similarly to the Legendre Polynomials, are the solution of the General Legendre equation

$$\frac{d}{dx} \left[(1 - x^2) \frac{d}{dx} P_l^{(m)}(x) \right] + \left[l(l+1) - \frac{m^2}{1 - x^2} \right] P_l^{(m)}(x) = 0.$$

The indices l and m are referred to as the degree and order of the associated Legendre function respectively. This equation has solutions that are nonsingular on $[-1, 1]$ only if l and m are integers with $0 \leq m \leq l$, or with trivially equivalent negative values. When m is even, the function is a polynomial. When m is zero and l integer, these functions reduce to the Legendre Polynomials.

In general, they can be considered as the m -th derivative of the Polynomial of order l , according to:

$$P_l^{(m)}(x) = (-1)^m (1 - x^2)^{m/2} \frac{d^m}{dx^m} (P_l(x)). \quad (24)$$

The Spherical Harmonics I

In mathematics, the Spherical Harmonics are the angular portion of an orthogonal set of solutions to Laplace's equation represented in a system of spherical coordinates:

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \varphi^2} = 0.$$

For $f(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi)$, the angular portion of Laplace's equation satisfies

$$\frac{\Phi(\varphi)}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{\Theta(\theta)}{\sin^2 \theta} \frac{d^2 \Phi}{d\varphi^2} + l(l+1)\Theta(\theta)\Phi(\varphi) = 0,$$

resulting, by making use of the technique of separation of variables:

$$\frac{1}{\Phi(\varphi)} \frac{d^2 \Phi(\varphi)}{d\varphi^2} = -m^2$$

$$l(l+1) \sin^2(\theta) + \frac{\sin(\theta)}{\Theta(\theta)} \frac{d}{d\theta} \left[\sin(\theta) \frac{d\Theta}{d\theta} \right] = m^2.$$

The Spherical Harmonics II

The angular solutions can be shown to be products of trigonometric functions and Associated Legendre Functions

$$Y_l^m(\theta, \varphi) = N e^{im\varphi} P_l^{(m)}(\cos \theta),$$

where Y_l^m is called a Spherical Harmonic Function of degree l and order m , $P_l^{(m)}$ is the Associated Legendre Function and N is a normalization constant. It is worth noticing that l represents the total number of nodal circles in the distribution: $l - m$ latitudinal and m longitudinal.

The most common normalization in physics leads to Spherical Harmonics Functions of the form

$$Y_l^m(\theta, \varphi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^{(m)}(\cos \theta) e^{im\varphi}, \quad (25)$$

which guarantees their orthonormality by

$$\int_{\theta=0}^{\pi} \int_{\varphi=0}^{2\pi} Y_l^m Y_{l'}^{m'}{}^* d\Omega = \delta_{ll'} \delta_{mm'}.$$

The Spherical Harmonics III

In neutron transport, the cylindrical symmetry of collision events with respect to the direction of the Center of Mass velocity, suggests the simplification of the problem by neglecting the dependence from φ , thus by assuming $m = 0$. The Spherical Harmonics Functions become then

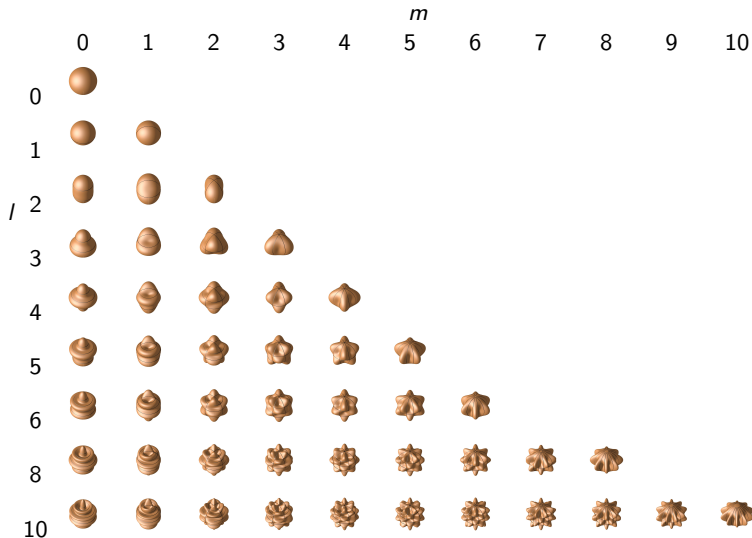
$$Y_l(\theta) = \sqrt{2l+1} P_l(\cos \theta),$$

with the orthonormality condition

$$\int_{\theta=0}^{\pi} Y_l Y_{l'} d\theta = \delta_{ll'}.$$

A visual representation of Spherical Harmonics distribution is given in the following figure, for several values of l and all the corresponding admitted values of m .

The Spherical Harmonics IV



Triangularization of the Coefficient Matrix I

The transformation $\mathcal{T}$ for the triangularization of the coefficient matrix $\underline{A}$ corresponds to a transformation operator $\underline{S}$ so that

$$\mathcal{T}(\underline{A}) \equiv \tilde{\underline{A}} = \underline{S}\underline{A}.$$

The transformation can be considered a succession of elementary operations, each of which acts on a pivot element in the main diagonal (i.e.: $a_{i,i}$), for the zeroing of the non-diagonal elements in the respective lower column ($a_{j,i}$, $j > i$). The matrix form of each elementary operation, $\underline{L}_i$, is thus

$$\underline{L}_i = \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 1 & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & -\frac{a_{N-1,i}}{a_{i,i}} & \dots & 1 & 0 \\ 0 & \dots & -\frac{a_{N,i}}{a_{i,i}} & \dots & 0 & 1 \end{pmatrix}.$$

Triangularization of the Coefficient Matrix II

The transformation operator $\underline{S}$ results therefore by the composition of the elementary transformation matrices to be ordinally applied on the left to the transforming coefficient matrix:

$$\underline{S} = \underline{L}_{N-1} \underline{L}_{N-2} \cdots \underline{L}_1 .$$

Convergence of Numerical Problems I

The convergence of the Jacobi method will be studied, since it represents the basis for the Gauss-Seidel and SOR methods too. The exact solution of the Jacobi problem, rewritten as

$$\vec{\Phi} = \underline{E}\vec{\Phi} + \vec{q},$$

where $\underline{E} = \underline{D}^{-1}\underline{C}$ and $\vec{q} = \underline{D}^{-1}\vec{b}$, is

$$\vec{\Phi} = (\underline{I} - \underline{E})^{-1}\vec{q}.$$

The iterative solution of the problem yields (assumed $\vec{\Phi}^{(0)} = \vec{0}$), to the following succession of vectors:

$$\vec{\Phi}^{(1)} = \vec{q}$$

$$\vec{\Phi}^{(2)} = \underline{E}\vec{\Phi}^{(1)} + \vec{q} = \underline{E}\vec{q} + \vec{q}$$

$$\vec{\Phi}^{(3)} = \underline{E}\vec{\Phi}^{(2)} + \vec{q} = \underline{E}^2\vec{q} + \underline{E}\vec{q} + \vec{q}$$

...

$$\vec{\Phi}^{(\ell)} = \underline{E}\vec{\Phi}^{(\ell-1)} + \vec{q} = \underline{E}^{\ell-1}\vec{q} + \underline{E}^{\ell-2}\vec{q} + \dots + \vec{q}.$$

Convergence of Numerical Problems II

It's easy to see that the convergence of the series is consistent with the analytical solution (i.e.: the equality $\vec{\Phi}^{(\infty)} = \vec{\Phi}$ holds) if and only if $\|\underline{E}\| < 1$:

$$\sum_{\ell=0}^{\infty} \underline{E}^{\ell} = \frac{1}{\underline{I} - \underline{E}} \iff \|\underline{E}\| < 1.$$

This condition leads to the progressive reduction of the error, defined as the distance of the temporary solution from the analytical one:

$$\vec{\varepsilon}^{(\ell)} \equiv \vec{\Phi} - \vec{\Phi}^{(\ell)} = \underline{E} \vec{\varepsilon}^{(\ell-1)}.$$

It can be shown that the iterative process is convergent if and only if the spectral radius of matrix $\underline{E}$ (i.e.: the radius of the smallest circle in the complex plane, centered in the origin, which contains all the eigenvalues λ_i of the matrix $\underline{E}$) is lower than unity:

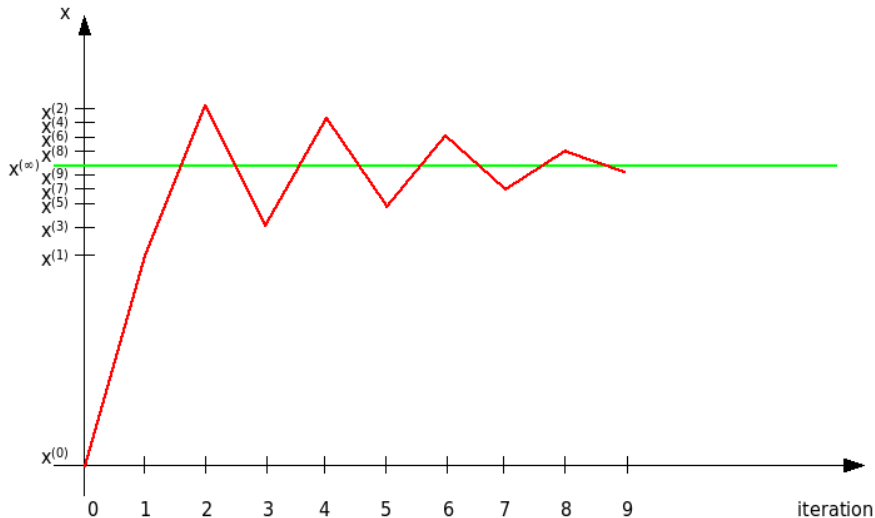
$$\rho_{\underline{E}} \equiv \max |\lambda_i| < 1. \quad (26)$$

Convergence of Numerical Problems III

A visual representation of the convergence of an iterative method is shown in figure. At every iteration the temporary solution is refined, according to two phases: an initial phase in which the temporary solution approaches monotonically the analytical one, starting from the initial tentative value (assumed $\vec{0}$ in figure), and a successive phase during which the evaluated solution oscillates around the analytical one, progressively reducing its distance from the latter.

The number of iterations needed to complete the first phase depends on both the coefficient matrix and the initial tentative value; on the other hand, the convergence of the temporary solution towards the analytical one only depends on the convergence properties, intrinsic of the coefficient matrix eigenspace.

Convergence of Numerical Problems IV



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