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DEVELOPMENT AND PERFORMANCE OF THE ANALYTIC NODAL DIFFUSION SOLVER "*ANDES*" IN MULTIGROUPS FOR 3D RECTANGULAR GEOMETRY

Juan-Andrés Lozano, José M. Aragonés & Nuria García-Herranz
Department of Nuclear Engineering; Universidad Politécnica de Madrid
c/ José G. Abascal, 2; 28006 Madrid (Spain)
lozano.jandres@gmail.com; arago@din.upm.es; nuria@din.upm.es

ABSTRACT

The Analytic Coarse-Mesh Finite-Difference method is developed in detail for multi-group and multi-dimensional diffusion calculations, including the general and particular modal solutions in the complex space for any number of groups. For rectangular multi-dimensional geometries, the Chao's generalized relations with transverse integration provide a high-order approximation of the ACMFD method, where all energy groups are coupled by matrix-vector FD relations and the errors are limited to the ones incurred by the interpolation of the transverse interface currents, in a non-linear iterative scheme. The implementation of the method in a multigroup 3D rectangular geometry nodal solver called *ANDES* is discussed, pointing out the encapsulation achieved for integration of the solver as an optional module within larger code systems. The performance of the ANDES solver in 3D rectangular (X-Y-Z) geometry and multi-groups is verified by its application to several 2D-3D model and international benchmarks (NEA-OECD), with given diffusion cross section sets in few-groups (2 to 8). The extensive verification, always required for new methods and codes, shows a quite fast convergence of ANDES in both the eigenvalue and transverse leakage iteration loops and with the nodal coarse-mesh size, allowing to reach the conclusion that quite high accuracy is achieved with rather large nodes, one node or four nodes per PWR fuel assembly, as compared with reference solutions obtained with fine-mesh finite-difference diffusion calculations using mesh sizes 64 to 128 times smaller than the ANDES nodes.

Key Words: nodal diffusion solvers, analytical methods, multigroup multidimensional neutron diffusion, nodal coarse-mesh finite difference.

1. INTRODUCTION

Few years ago, the Analytic Coarse-Mesh Finite-Difference Method (ACMFD) of Chao [1] was fully developed and implemented for two-group and two-dimensional diffusion calculations in our own code system for PWR core analysis [2]. The performance demonstrated in the 2D rectangular X-Y case and 2-group implementation was excellent, and represented the "proof-of-principle" of the ACMFD method possibilities. Recently, and following the same guidelines, the ACMFD methodology has been extended for multigroup and multidimensional problems [3].

In this work, we address the implementation of this methodology in a new 3D *A*nalytic *N*odal *D*iffusion *S*olver called *ANDES*. This first version of *ANDES* is restricted Cartesian 3D geometry

and steady-state k-eigenvalue calculations in any number of energy groups; thus it mainly addresses PWR and BWR steady-state core simulations. The problems and particularities found in the generalization of the ACMFD method −to 3D and any number of groups− are discussed, such as the frequent appearance of complex (conjugate) eigenvalues and eigenfunctions or the difficulty of the transverse leakage accurate treatment. The performance and verification of the solver are shown for a set of 2D and 3D model and full-core international benchmarks.

2. THE ANALYTIC MULTIGROUP DIFFUSION THEORY

2.1 Decoupling of the multigroup diffusion equations

When we try to solve the set of G (number of groups) multi-group diffusion equations inside a homogenized region, we find that they are coupled by the terms of fission in thermal groups releasing neutrons at fast groups, and the scattering terms, both down-scattering and up-scattering. The equations can be expressed in a vectorial form, this way:

$$\nabla^2 |f(\boldsymbol{r})\rangle - \boldsymbol{A}\,|f(\boldsymbol{r})\rangle = -\boldsymbol{D}^{-1}|\boldsymbol{S}(\boldsymbol{r})\rangle \tag{1}$$

Where $\boldsymbol{A}$ is called the multi-group diffusion matrix and includes the absortion, fission and scattering terms of the balance. The fluxes are in *ket*-notation, representing the column-vector of G group fluxes. Also the external source distribution *S* is expressed with this notation.

The way to solve the coupled linear system is to **diagonalize** the matrix $\boldsymbol{A}$ which is non-singular so it can be written as follows:

$$\boldsymbol{A}|\boldsymbol{u}_m\rangle = l_m|\boldsymbol{u}_m\rangle \;;\; \boldsymbol{R}^{-1} = [\boldsymbol{u}_m] \;;\; \boldsymbol{A} = \boldsymbol{R}^{-1}\,[l_m]_{\text{diag}}\boldsymbol{R} \tag{2}$$

Where l_m and u_m are the eigenvalue and eigenvector for mode *m.* Thus, pre-multiplying equation (1) by matrix $\boldsymbol{R}$ and assuming that:

$$|y_m\rangle = \boldsymbol{R}|f_g\rangle \;;\; |f_g\rangle = \boldsymbol{R}^{-1}|y_m\rangle \;;\; |\boldsymbol{s}_m\rangle = \boldsymbol{R}\boldsymbol{D}^{-1}|\boldsymbol{S}_g\rangle \;;\; |\boldsymbol{S}_g\rangle = \boldsymbol{D}\boldsymbol{R}^{-1}|\boldsymbol{s}_m\rangle \tag{3}$$

The G multigroup coupled equations (1) are reduced to another G uncoupled *modal* equations. Solutions for these equations are the *modal fluxes* which are related to the physical fluxes by a linear relation (3).

$$\nabla^2 y_m(\boldsymbol{r}) - l_m\, y_m(\boldsymbol{r}) = -\boldsymbol{s}_m(\boldsymbol{r}) \quad ; \quad m = 1, \mathrm{G} \tag{4}$$

2.2. The ACMFD method for 3D Cartesian problems

2.2.1. Transverse Integration

The Analytic Coarse Mesh Finite Difference nodal method for the 1D diffusion equation is exact. So in order to approximate our 3D solution to the 1D reference, one way is to perform a Transverse Integration of either equation (1) or equation (4). The result of this integration is:

$$S_g^{*}(x) = S_g(x) + \left[J_y^{-H_y/2}(x) - J_y^{+H_y/2}(x)\right]/H_y + \left[J_z^{-H_z/2}(x) - J_z^{+H_z/2}(x)\right]/H_z \tag{5}$$

$$\frac{d^2\left|y_m(x)\right\rangle}{dx^2} - l_m\left|y_m(x)\right\rangle = -\boldsymbol{R}\,\boldsymbol{D}^{-1}\left|\boldsymbol{S}_g^{*}(x)\right\rangle \tag{6}$$

Consequently we obtain an equation for the integrated 1D-dependant flux. This equation would provide the analytic distribution for the 1D-flux if the 1D distribution of the external source (including transverse leakage) were known. However, as it will be seen later, it is impossible to know the real 1D distribution of currents in a nodal scheme, so there will always be an error associated to the profile that we fit to approximate this distribution.

2.2.2. Solution of the modal equation in 1D with sources. Chao's relation

The ACMFD relation gives an expression for the flux at the interfaces in terms of the average flux at the adjacent node and of the current at the same interface. This relation comes from the analytic solution for equation (6):

$$y_m(x) = A_m e^{+a_m x} + B_m e^{-a_m x} + p_m(x)\ ;\ \frac{d^2}{dx^2}p_m(x) - l_m\ p_m(x) = -s_m(x)\ ;\ a_m = \sqrt{l_m} \tag{7}$$

Determining the constants A_m and B_m from the values of flux and current on interfaces:

$$y_m(\mp\frac{H}{2}) - p_m(\mp\frac{H}{2}) = C_m^{\,f}\left[\overline{y}_m - \overline{p}_m\right] \pm C_m^{\,j}\frac{H}{2}\left[J_m(\mp\frac{H}{2}) + p'_m(\mp\frac{H}{2})\right] \tag{8}$$

Where C^f and C^j are constants for every mode and depends only on the eigenvalue (it is on XS's) and on the nodal length over the analyzed direction.

$$C_m^{\,f} = \frac{2\,a_m H}{e^{+a_m H} - e^{-a_m H}}\quad ;\quad C_m^{\,j} = \frac{e^{+a_m H} + e^{-a_m H} - 2}{e^{+a_m H} - e^{-a_m H}}\frac{2}{a_m H} \tag{9}$$

Finally, transforming from the modal fluxes to the physical group fluxes, using (3), we obtain:

$$\left|f_g(\mp\tfrac{H}{2})\right\rangle = \boldsymbol{A}^f\left|\overline{f}_g\right\rangle \pm \frac{H}{2}\boldsymbol{A}^j\boldsymbol{D}_g^{-1}\left|\boldsymbol{J}_g(\mp\tfrac{H}{2})\right\rangle - R^{-1}\left|\boldsymbol{T}_m(\mp\tfrac{H}{2})\right\rangle \tag{10}$$

$$\boldsymbol{A}^f = \boldsymbol{R}^{-1}\boldsymbol{C}^f\boldsymbol{R}\ ;\quad \boldsymbol{A}^j = \boldsymbol{R}^{-1}\boldsymbol{C}^j\boldsymbol{R} \tag{11}$$

The particular modal solution involved in relation (10), in term $\boldsymbol{T_m}$, has an important role in obtaining an accurate solution, as it gathers all the error associated to the approximations. This column-vector includes all the terms related to the particular solution given in (8).

2.2.3. Limitation of the ACMFD relation

Attending to expression (9), namely to the denominator of the modal scalars $C_m^{\,f}$ and $C_m^{\,j}$, we see that the unique possibility to be equal zero is that argument $a_m H = ip$ (issue already discussed in [4]). Of course if $a_m H = 0$ the denominator is zero, but also the numerator, and we have an indetermination 0/0. In this case if we obtain that:

$$\lim_{g\to 0} C_m^f = 1 \; ; \; \lim_{g\to 0} C_m^j = 1 \; ; \; g = a_m H \tag{12}$$

Then the ACMFD relation only may fail when $a_m H = ip$, which only occurs with the fundamental mode in supercritical nodes. Given that a_m only depends on nodal cross sections and K_{eff} we have to assure that our iterative process doesn't reach this condition by two different procedures:

- To initialize the outer iteration with high values of K_{eff}, because initial values excessively low lead to more negative fundamental eigenvalues.
- To use a nodal width sufficiently fine. With real scale cores there are no problems with fuel assembly size nodes. Nodal width must be lesser than the half of the minor characteristic lengths of the core.

2.2.4. Particular solution per direction and node

Since the equation we are trying to solve (4) is a non-homogeneous one, solution has a heterogeneous term. The effective external source of equation (4) is not only a real external source $S_g(x)$ but in addition the transverse leakage at faces parallel to our direction $L_y(x)+L_z(x)$.

The problem is that we can't guess the distribution of transverse leakage as it is part of the solution. Thus in ANDES as in other nodal solvers it is chosen a polynomial interpolation for this function. This code has the option of choosing among *Flat*, *Parabolic* or *Cubic* fit, being the first much less accurate than the others.

3. IMPLEMENTATION IN THE *ANDES* SOLVER

The ACMFD formulation has been implemented in the *ANDES* solver following the scheme shown in Figure 1, for steady-state calculations for the time being. The code, written in Fortran 77-95, using the Intel and GNU Linux compilers, is composed of a set of subroutines oriented to execute the different tasks involved in the calculation. Moreover, attention to data flux management has been an important issue, in order to:

1. Optimize the memory management, with flexible dimensioning of data in dynamical and static storage.

2. Encapsulate the *ANDES* solver, with well defined interface variables (input and output), to provide the capability to integrate the solver in other code systems, having different data structure. In fact, the integration has already been done in our own code (*COBAYA3*) [5] and in the *DESCARTES* platform [6], in the framework of the European *NURESIM* project.

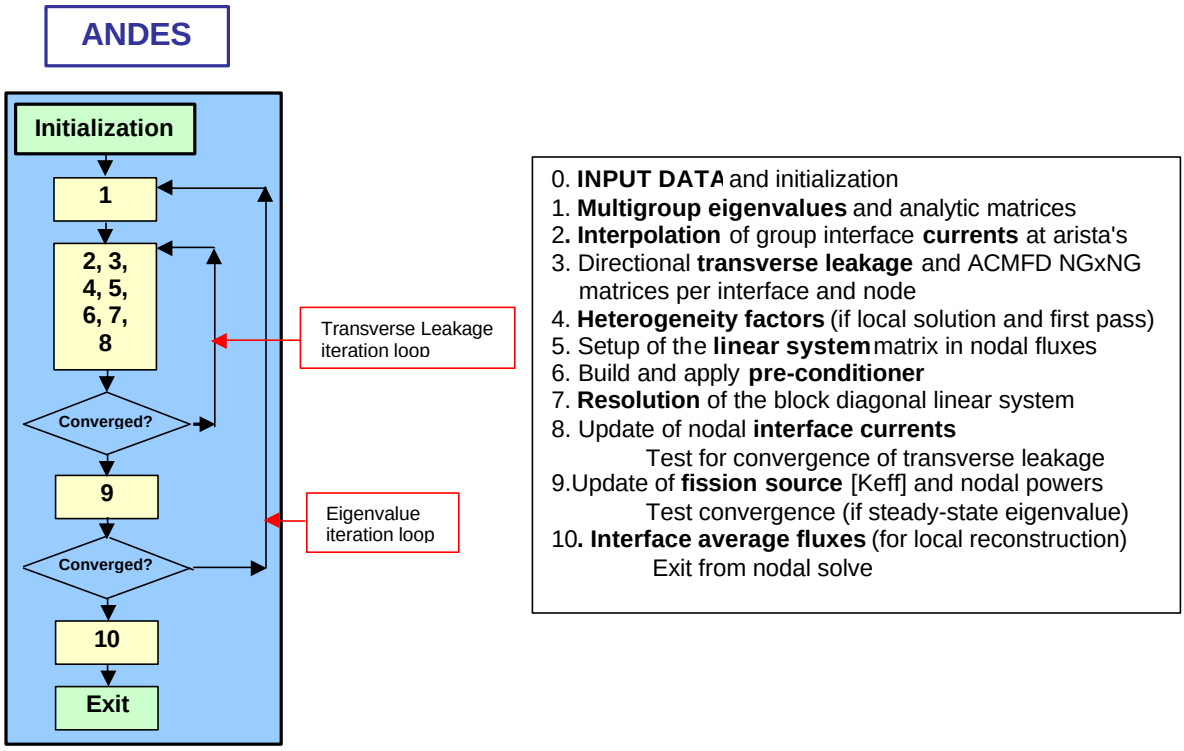


Figure 1. *ANDES* iterative solution scheme

4. RESULTS

An extended set of benchmarks has been performed during the process of *ANDES* verification, ranging from tests of self-consistency with mesh refinement to the verification of the code with some of the full-core steady state NEA benchmarks. This paper includes an overview of results obtained for these benchmarks, analyzing the factors relevant for the accuracy of the solution.

The first benchmark with a simple spatial definition is appropriated to show the importance of the transverse leakage approximation in the formulation. The second one is a full core benchmark [7] to verify the agreement of the calculations with the reference results and to analyze computing time in a 3D 2 group solution. Finally we introduce the PWR MOX/UO_2 core benchmark [8] which has 2, 4 and 8 group cross section libraries allowing us to analyze diffusion solutions in more than 2 groups. Besides this benchmark is used to show how *ANDES* has been successfully coupled with the thermalhydraulic code *COBRA III* [9].

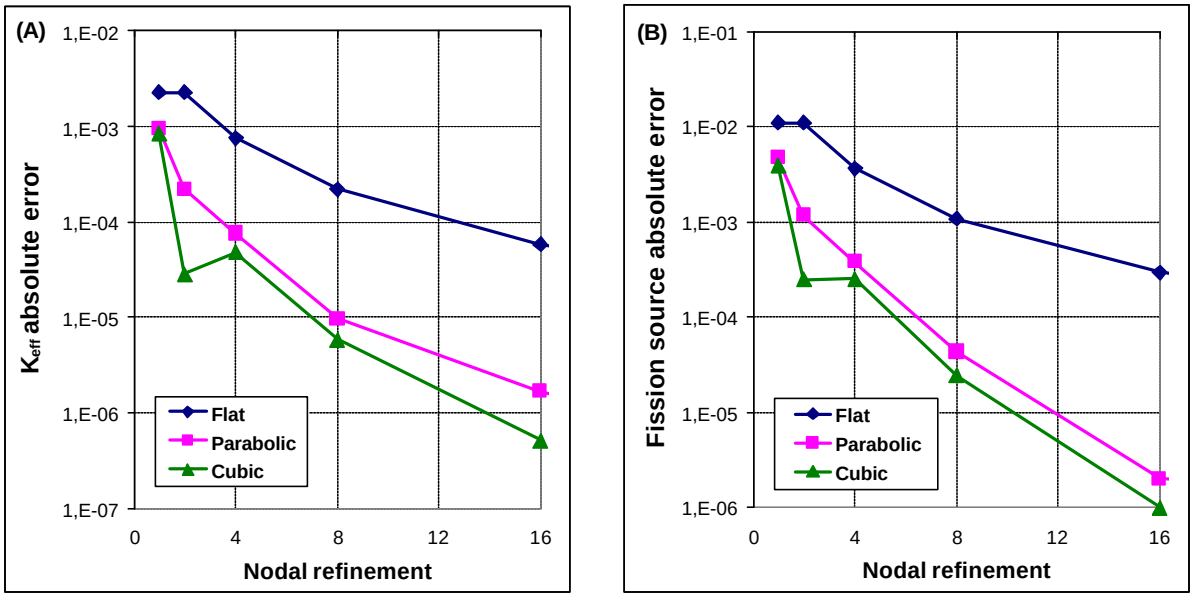
4.1 PWR 2D model color-set benchmark

As it was explained in the description of the ACMFD method at chapter 2, the 1D transverse integrated diffusion equations have an independent term whose distribution is not known because the interface current profile is not available in a nodal scale solver. Then, the unique way to obtain accurate results is to perform the best interpolation of our average nodal interface currents in order to fit in the real profile. The most usual in nodal solvers is the polynomial interpolation

within a node face, using the average currents of the face and its two adjacent ones, due to the low computational cost and the easiness of the analytic solution of equations.

With *ANDES* we can choose from *Flat*, *Parabolic* or *Cubic* interpolations. A good way to test the effect of the transverse leakage (T.L.) approximation on the results is to simulate a model "*color-set*", which is a two media with chessboard distribution (1=fuel; 2=fuel+absorber) and reflective boundary conditions.

Figures 2A and 2B shows the solution in 2 groups with a set of typical PWR fuel cross sections and 20 cm fuel assembly width. The error in both the eigenvalue and the normalized fission source at assembly 1 are analyzed for *Flat*, *Parabolic* and *Cubic* T.L. interpolation, with different nodal refinement degrees.



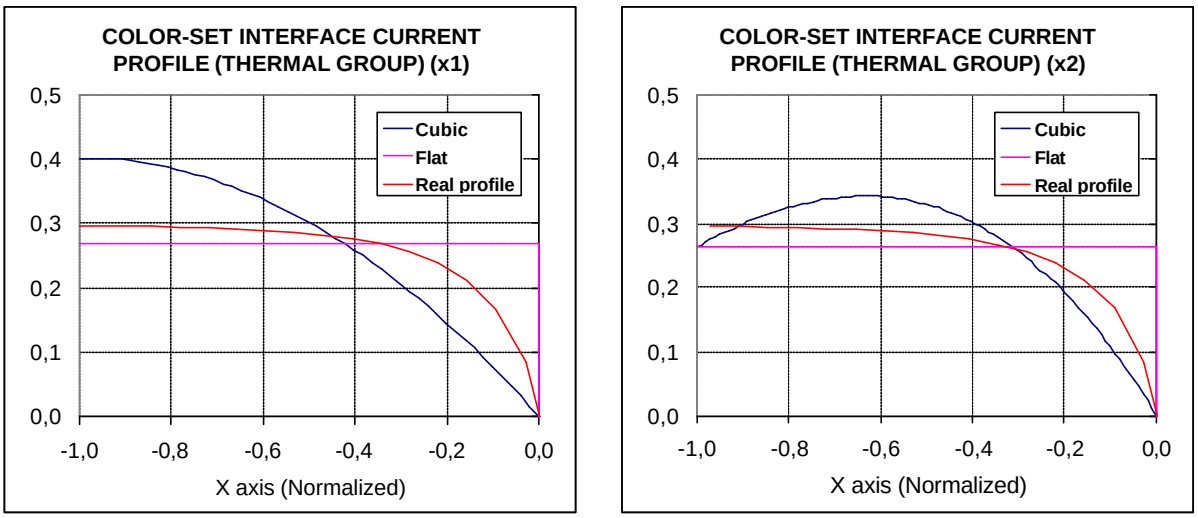
Figures 2A and 2B. Absolute error both in K_{eff} (A) and in normalized Fission Source per assembly (B), respect to converged solution: *cubic* (x32)

The aim of this comparison is to show that the only source of error in a solver based on ACMFD theory for diffusion is in the difference between the real profile of transverse leakage and the polynomial fit.

We find that the *cubic* and *parabolic* fits are more than one order of magnitude more accurate than the *flat* approximation, so we could take a fourfold wider mesh, obtaining the same precision. Furthermore using the *cubic* and *parabolic* interpolation does not increase the computing time because of the low amount of instructions needed for this task. However using a *cubic* fit instead of a *parabolic* one leads to near similar solutions.

The role of the T.L. profile in the solution accuracy is determinant. In this case, the profile is given by the current at the centreline of the color-set. The following Figures 3A and 3B show this profile compared to the different approximations for 2 nodal refinements (x1 and x2). The x

axis goes from one centre of assembly interface (-1) to the central corner (There is symmetry for the rest of the interface).



Figures 3A and 3B. Transverse current profiles for flat and cubic interpolations with 1x1 node (A) and 2x2 nodes (B) per fuel assembly (PWR).

It can be seen that *Flat* approximation overestimates T.L. near of the assembly edge (x=0) and underestimates it at the assembly centre. As a result, interface average currents are increased and so the ratio between average fluxes at both regions and the K-effective are also increased respect to the authentic values. With *Cubic* interpolation the effect is the contrary so K_{eff} eigenvalue is smaller than the authentic one. The *parabolic* interpolation is quite close to the *cubic* one.

4.2. NEA-NSC 3D PWR core transient benchmark, uncontrolled withdrawal of control rods at zero power

ANDES code has been tested with several PWR steady-state benchmarks to verify its performance with full core cases. To this end we have selected two initial steady states proposed for the 2-group benchmark defined by Roger Fraikin & Herbert Finnemann [7].

Basically it consists on a 157-fuel elements core with a layer of reflector elements surrounding it. Axially it has 16 nodal layers and lower and upper reflector nodes. The two initial steady states correspond to a HZP state and different configuration of control banks (A, B, C, D, and S):

Steady State 1: Bank D inserted, other banks are fully withdrawn.
Steady State 2: Banks A, B, C, D inserted, shutdown banks withdrawn.

For both cases the *ANDES* results (using 1x1 and 2x2 nodes per element) are compared with the reference results given by the Nodal Diffusion Code *PANTHER* (using 3x3 nodes per element) in Table I below.

Table I. Comparison and results of NEA-NSC PWR core benchmark

CASE	Critical Boron (ppm error)		F_Z (Relative error %)		F_{XY} (Relative error %)	
	1x1	2x2	1x1	2x2	1x1	2x2
S. state 1	3,4	-0,3	-0.07	-0,07	-0,81	0,08
S. state 2	1,1	-0,3	-0,07	-0,07	-0,31	-0,15

Up to now no mention has been done about the convergence of the resolution method and the computing time. This is not the main issue of the paper so that only a brief overview is included. Regarding to convergence, *ANDES* solver uses a Bi-CGSTAB algorithm to solve the linear system which has proved to be robust enough in all range of cross sections and geometry employed for different benchmarks. For the K_{eff} iterative calculation the Wielandt method has been implemented achieving high reduction in total outer iterations (typically 18-25 iterations for full 3D cores). Figure 4 shows the evolution of absolute error both in K_{eff} and Fission source during the iterative process in **steady state 1** for 1x1 and 2x2 nodes per fuel assembly.

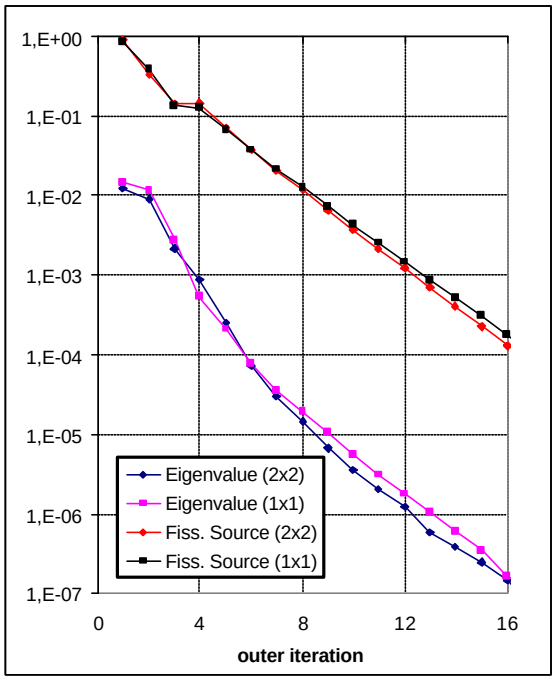


Figure 4. Convergence rate in K_{eff} and fission source for 3D core benchmark

Concerning the computing time, it is considered that *ANDES* solver is still at optimization phase, so this issue may improve in further developments. Focusing on this benchmark, in the table below there are values corresponding to several nodal resolutions. The time fractions employed in the main computing tasks are also included.

Table II. Computing time for 3D NEA-NSC PWR core benchmark

	Steady state 1		Steady state 2	
	1x1	2x2	1x1	2x2
Total time (s)	4.9	20.9	5.0	22.0
Eigenvalues & eigenvectors (%)	16,1	13,8	16,1	13,8
Linear system coefficients (%)	37,1	34,7	37,0	35,3
Preconditioning (%)	27,6	24,1	27,4	24,1
Bi-CGSTAB (%)	**16,5**	**24,9**	**16,8**	**24,3**
Interface currents (%)	2,7	2,5	2,7	2,5

From the values of the table we conclude that computing time fraction for linear system resolution increases more than proportionally with the total number of nodes, so perhaps more effort in preconditioning is needed, but total computing time is nearly proportional to the number of nodes.

This benchmark also has been the object of more verification tasks. A 2D version of **steady state 1** was implemented to compare results with those given by our pin-level Diffusion code *COBAYA3* which has been run assuming homogeneous assemblies. Thus the comparison focuses on mesh width error. Assembly refinements were 1x1, 2x2 and 3x3 nodes per assembly (4x4 is the reference) in *ANDES* and 17x17, 34x34 and 68x68 cells per assembly in *COBAYA3*.

Table III. 2D full core verification with pin-level Diffusion code *COBAYA3*

Refinement	K-eff (diff. with * in pcm)		F_{XY} (relative error in %)	
	ANDES	*COBAYA3*	*ANDES*	*COBAYA3*
1	1,004166 **(36,2)**	1,004298 **(49,4)**	1,2334 **(0,96)**	1,2349 **(0,84)**
2	1,003820 **(1,6)**	1,003957 **(15,3)**	1,2439 **(0,11)**	1,2427 **(0,21)**
3	1,003802 **(-0,2)**	1,003851 **(4,7)**	1,2449 **(0,03)**	1,2445 **(0,06)**
4	1,003804 **(*)**		1,2453 **(*)**	

4.3. OECD/NEA and U.S. NRC PWR MOX/UO_2 core benchmarks

It was considered interesting to run this set of benchmarks because it allows us to extend the verification of the *ANDES* solver from 2 groups up to 8 groups, furthermore it includes an ADF library so we could also test the heterogeneity treatment.

An important development in the process of *ANDES* implementation has been its coupling with a thermalhydraulic code to enable the simulation of steady states at HFP. Namely we have used the LWR thermalhydraulic code *COBRA III*. For this benchmark a 3D core has been defined with a set of cross sections interpolated both in moderator density and Doppler temperature.

The coupling has been done with 1 or 4 nodes (*ANDES*) and 1 or 4 channels (*COBRA III*) per fuel assembly. Obtained results are compared in Table IV to those provided by PSU — *PARCS* code for 2 groups— 3D diffusion and 2x2 nodes per fuel assembly. In absence of reference results for 8 groups, the analysis is a self-comparison with 2 group solution.

This benchmark considers a 3563 MW core with 193 UO_2 / MOX fuel assemblies. The focus by now will be on the steady state defined by the following parameters:

State: All Control Rods Out, 1/8 symmetry.
Hot Full Power conditions (Power=100%, P_{in}=15.5 MPa, T_{in} = 560 K)

Table IV. Comparison results of 3D PWR MOX/UO_2 core benchmarks

Critical Boron (ppm error)		F_Z (Relative error %)		F_{XY} (Relative error %)	
1x1	2x2	1x1	2x2	1x1	2x2
1691,2 **(11,9)**	1688,9 **(9,6)**	1,418 **(0,07)**	1,418 **(0,07)**	1,368 **(-0,15)**	1,375 **(0,36)**

A critical boron search is performed within the thermalhydraulic iteration loop. During this iteration an adaptive convergence criteria in K_{eff} (*ANDES*) has been implemented in order to reduce the total computing time. The idea is to make the convergence in K_{eff} dependant on the variation of power distribution respect to the previous iteration one. This way, computing time decreases in the first iterations. In Figure 5 we plot the normalized change in power distribution, and in boron concentration and the K_{eff} criteria for *ANDES* calculation. This last one is the same in the two first iterations because the algorithm is based on the power distribution of the previous iteration.

To test the self-consistency of the ANDES calculations with different number of groups, Table V shows the results obtained for the 2D HZP case of the same benchmark with two different spatial refinement (1x1 and 2x2 nodes per assembly) and different number of groups.

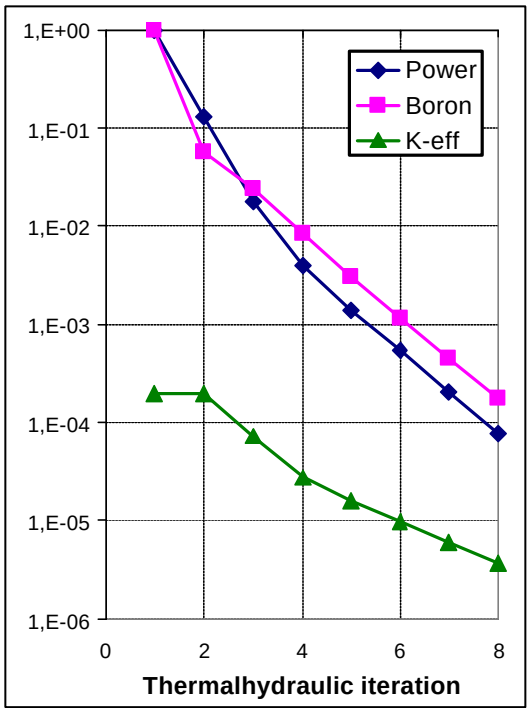


Figure 5. Adaptive convergence of ANDES coupled with TH code

State: All Control Rods Out, 1/8 symmetry.
Hot Zero Power conditions (ρ_m = 752.06 kg/m3, T_{core} = 560 K, Boron = 1000.0 ppm)

Table V. PWR 2D MOX/UO_2 benchmarks: Verification of Multi-group formulation

	Mesh	Number of Groups		
		2	**4**	**8**
K-eff Pcm diff. (8g 2x2)	1x1	1,063811 **-8,7**	1.063862 **-3,6**	1.063930 **+3,2**
	2x2	1,063792 **-10,6**	1,063837 **-6,1**	1,063898 **Ref.**
Computing time (s)	1x1	0,340	0,631	1,382
	2x2	1,432	2,646	5,496

The table above shows that (1x1) computation suppose an increasing of about 2 or 3 pcm's respect (2x2) calculation, regardless of the number of energy groups. There is also a good agreement between results obtained with 2, 4 and 8 groups, with differences below 11 pcm's. Computing time increases linearly with the number of groups, which is a good result given that the unknowns are twice when we double the number of groups.

5. CONCLUSIONS AND ONGOING WORK

Verification of performance has shown that *ANDES* is a code with higher order definition, both in neutron energy and spatial distribution, respect to our previous available codes, as it goes from two-group and two dimensions to any number of groups and three dimensions, while the computing time is kept proportional to the number of unknowns (nodes-groups). It can perform calculations standing alone by using nodal cross sections and discontinuity factors libraries (which is the subject of this paper) or it can be executed as an accelerating module in coupled calculation with the pin-scale diffusion code *COBAYA3* [5].

The set of tests taken in *ANDES* verification process have shown the high convergence rates, in terms of mesh refinement, of a code based on the ACMFD formulation. In general, with 1x1 nodes per fuel assembly K_{eff} absolute error is below 50 pcm and maximum assembly fission source error is below 1%, and for 2x2 nodes per assembly these values decrease to 2 pcm and 0,2%. The most remarkable of these results is that *ANDES* formulation achieves (with 2x2 nodes per assembly) a level of accuracy such that a standard fine-mesh finite-difference scheme would need 136x136 cells per assembly.

The ongoing work in the framework of *ANDES* includes the development of additional computational capabilities and improvements, in process of implementation and verification, namely: Ongoing work address additional capabilities and improvements, including a full analytic scheme for heterogeneous nodes with part control or continuous changing intra-nodal properties (such as TH or burnup); neutron kinetics and coupling to core thermal-hydraulics for source and transient problems; and 3D triangular-Z geometries for VVER, HTR and fast reactors.

- Testing of a new full analytic scheme, consistent with the ACMFD method, for treating heterogeneous nodes, with control rods partially inserted (to reduce the effect known as *rod cusping*), continuously changing intra-nodal properties (such as TH or burnup), or strong discrete heterogeneities (MOX, burnable absorbers or control).
- Implementation of kinetics terms in nodal coupling and balance equations of the ACMFD method to enable the consistent simulation of transient and source problems, initialized from steady states and driven by the modification of neutronic or thermalhydraulic parameters (control assemblies, boron, inlet coolant temperature, flow, etc).
- Adaptation of the ACMFD method to 3D triangular-Z geometry to allow the simulation of hexagonal lattice fuel assemblies and cores in VVER, HTR and fast reactors.

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