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SIMMER Extension for Multigroup Energy Structure Search using Genetic Algorithm

M. Massone, F. Gabrielli, A. Rineiski

Karlsruhe Institute of Technology (KIT): Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany, D-76344, mattia.massone@kit.edu

Abstract – *The multigroup transport theory is the basis for many neutronics modules. A significant point of the cross-section generation procedure is constituted by the choice of the energy groups boundaries in the cross-section libraries, which must be carefully selected as an unsuitable energy meshing can easily lead to inaccurate results. However the decision can require considerable effort and is particularly difficult for the common user, especially if not well-versed in reactor physics. This work presents a tool based on a genetic algorithm which selects an appropriate cross-section energy structure specific for the considered problem, to be used for the condensation of a fine multigroup library. The procedure is accelerated by results storage and fitness calculation acceleration and can be easily parallelized. The extension is applied to the coupled code SIMMER and tested on the ESNII+ ASTRID-like reactor system. The results show that, when the libraries are condensed based on the energy structures suggested by the algorithm, the code actually returns the correct multiplication factor, in both reference and voided conditions. The computational effort reduction obtained by using the condensed library rather than the fine one has been assessed and is much higher than the CPU time required to perform the energy structure search.*

I. INTRODUCTION

SIMMER (1, 2) is a multi-velocity-field, multiphase, multicomponent, Eulerian fluid-dynamics code coupled with a space-dependent neutron transport kinetics model, primarily developed for safety studies on liquid-metal-cooled fast reactors. During the simulation, the neutronics module of SIMMER employs macroscopic cross-sections (XSs) with a broad-groups energy structure (ES) as input libraries, which are originally obtained from the point-wise libraries or by collapsing the reference libraries at several hundreds of energy groups available at KIT with a weighting function (neutron spectrum) specified by the user.

A code extension that allows including the collapsing procedure inside SIMMER has already been proposed (3). In this way the energy discretization of the XSs actually used in the transport calculation (referred as broad-groups libraries, BL) can be coarser than the one of the input libraries (hence denoted fine-libraries, FL). The XSs obtained from these libraries are collapsed at each time step with the advantage that the collapsing is done with neutron spectra obtained for the transient conditions in each core sub-region.

A particular difficulty for the user is the choice of the optimal broad-group ES to be used, which might have a significant impact on the results (3). Since no automatic tools are available to fulfill this goal, the choice of the optimal broad-group ES is left to the user, who must have good knowledge on neutronics and has often to perform investigations of the different options to avoid non-optimal or misleading solutions.

Having this in mind, the employment of an evolutionary genetic algorithm (GA) in the SIMMER environment is proposed in the paper in order to compute the most "proper" broad energy group discretization for transient analyses. Similar approaches, focused on swarm algorithms, have been followed in the past by Mosca et al. and by Yi and Sjoden for both single pins in thermal reactors (4, 5) and infinite homogeneous problems in fast systems (6).

The computational expense required by the GA is fully compensated by its advantage: by using the optimal ES for the XS collapsing it is possible to perform neutronics calculations having nearly the same accuracy as using the FL and the computational time of the BL. This advantage proves particularly important if the transport calculation must be repeated for a large number of times, as in the case of transient computations with SIMMER. Moreover, since the optimal ES is not expected to change significantly if the system geometry is not deeply altered, the GA must not be performed for each simulation of the same system. This work presents a complement to the XS collapsing extension for SIMMER (3), aiming to solve the ES search problem with a GA. The extension is then applied to the ESNII+ ASTRID case to demonstrate its effectiveness and to study the physics behind the results, also in case of voided conditions. Finally the computational expense is assessed and compared with the time reduction owing to using the BL rather than the FL.

II. DESCRIPTION OF THE ACTUAL WORK

GAs (7) are a widely used type of metaheuristics for search and optimization, based on the principles of Darwinian selection and evolution (on which the wider set of evolutionary algorithms is founded).

The starting point of a GA is a collection (using the analogy of biology, denoted by population) of possible solutions (individuals), characterized by a set of properties (genes), usually randomly generated; the members of the

population are tested and used to produce a new population (next generation), based on a measure of their adequateness as problem solution called "fitness". As the iterations go on the solution space is explored and the quality of the population grows, eventually approaching the optimal (or at least a reasonably reliable) solution, similarly to natural evolution.

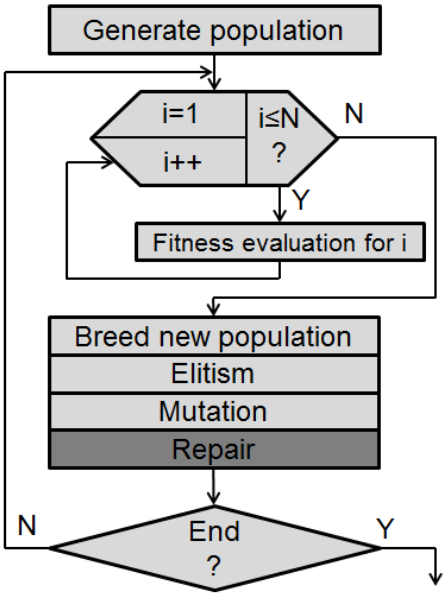

Fig. 1. GA flowchart. Repair block is specific for the current application due to the chosen chromosome representation.

1. Chromosome representation

The way of representing the individual genes set (chromosome) is highly problem-specific and is the first point to be addressed when setting a genetic algorithm up.

The specific constraints applicable to this case are two:

I. The gene pool is finite, i.e. the energy cuts of the BL can be set only just at the ones present in the FL;

II. The number of energy cuts to be set, i.e. the number of energy groups of the BL, is fixed *ab initio*.

A non-binary representation has been chosen, consisting of chromosomes with a number of genes *FG*-1; each gene can assume any integer value (allele) of the interval (1,*MG*], representing the first fine-group belonging to a broad energy group. It is implicit that the original and the collapsed libraries share the same starting energy. Constraint II can be enforced by making sure that each allele does not appear twice in the chromosome.

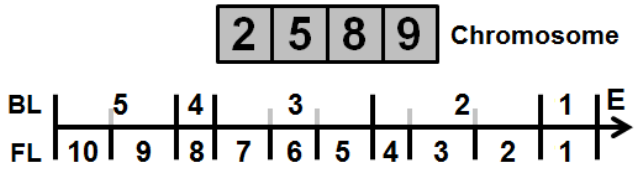

Fig. 2. Example of 5-groups BL collapsed from a 10-groups FL based on a chromosome.

Sorting of the genes based on their alleles has pros and cons; experience suggests that sorted chromosomes give better results.

2. Fitness function

As for any evolutionary algorithm, a fitness function (FF) is required to rank the solutions based on their suitability in solving the problem. This function represents in biological systems the reproductive success, at the base of natural selection and evolution.

Different options are possible, but the required computational expense should be taken into account, as the FF must be evaluated for each individual of each generation.

Similarly to Yi and Sjoden (4), a simple and suitable fitness function is considered to be

$$f_I = \left| k_{eff}^{(I)} - k_{eff}^{obj} \right| \cdot 10^5, \qquad (1)$$

where the objective k_{eff} can be easily identified performing an eigenvalue calculation with the original uncollapsed FL.

A. Computational expense reduction

As the alleles are chosen from a discrete set, there is quite a chance of examining twice the same individual. The probability of this occurring is actually much higher than predicted by simple combination counting, as each generation depends on the previous one. Repeating the evaluation of the fitness, of course, must be avoided to the utmost, as it is the most expensive operation of the GA. Hence a binary tree storage is implemented, keeping track of all explored configurations and of their fitness; the tree is searched for each individual before performing the eigenvalue calculation, which can be skipped if the required fitness is already known. The time spent in creating, keeping and deallocating the tree is amply compensated by the spared calculations.

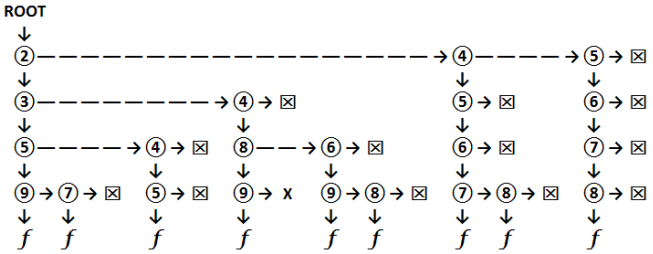

Fig. 3. Storage tree example for 9 to 5 groups collapsing.

Also, fitness estimation itself is accelerated: the eigenvalue calculation with the FL produces, along with the objective k_{eff}, the neutron fluxes with the uncollapsed ES. If these fluxes are collapsed (following each individual chromosome), with the formula

$$\phi_G = \sum_{g=C(G-1)}^{C(G)-1} \phi_g , \qquad (2)$$

they represent a well educated guess for the transport solver, which then is able to converge to the solution of the eigenvalue calculation within few iterations.

Finally, as each individual of a generation is completely independent from the others, the algorithm is very suitable for an efficient parallelization.

3. Genetic operators

As selection operator, the tournament method (8) is chosen, mainly for being easily tunable. The individuals selected with this method constitute the mating pool, from which couples are randomly extracted to create two offspring through one-point crossover (XO). When the reproduction phase is finished, the parents are all discarded (non-overlapping population model), with the exception of the best-performing ones, which are passed to the next generation unchanged (elitism).

Genetic diversity is improved by mutation: once the next generation is established, a fixed number of randomly chosen genes have their value replaced with another randomly chosen allele. This procedure improves the diversity of the genetic pool, may reintroduce extinct alleles and opposes to genetic drift.

A. Chromosome repair

The chosen representation stipulates that each allele appears in a chromosome at most once; nevertheless, after mutation or crossover such duplications can occur. Hence one requires a chromosome repair mechanism, which must not be too invasive, in order to avoid excessive perturbation of the natural selection process.

Therefore, after the new generation has been created, all individuals are checked for duplication errors. If such errors are observed, a mutation of the genes with duplicated alleles is performed, until all damaged chromosomes are fixed.

4. Test configuration

The aim of the test procedure is finding an ES with 11 energy groups starting from the 72-groups XS data libraries developed at KIT for SIMMER analyses (9) able to reproduce the reference results with respect to the criticality level and the Doppler and coolant reactivity feedbacks in a fast reactor system. The number of groups of the final ES, which can be defined by the user, has been chosen as most of the mechanistic calculations with SIMMER at KIT are performed using an 11-groups library (10).

A. Algorithm configuration

While for most applications a sub-optimal solution is probably sufficient to achieve good results, in this case the algorithm is configured with very tight parameters in order to achieve refined results, more suitable for the study of the position of the energy cuts.

Each generation is composed of 500 individuals, a large number intentionally chosen to limit the genetic drift effect.

The selection pressure is kept to a low level by using 100 tournaments without replacement (all individuals of the population participate in exactly one tournament) of the stochastic type, i.e. all participants of the tournament are included in the mating pool with a number of copies

$$M_I = (1-p)^{R_I - 1} \qquad (3)$$

with p=0.1.

Finally, 5% of the chromosomes of the next generation are mutated and the top-2% of each generation passes to the next one with the elitist mechanism.

Fifty generations are always examined, with anticipated interruption in case no improvements are obtained for 20 consecutive generations.

In order to reduce the stochastic effect in the results, the GA is carried out 5 times. The calculation has also been repeated 2 times more with the core in voided condition, in order to study the effects on the energy discretization on the feedback effect.

B. Test system description

The test system is the Advanced Sodium Technological Reactor for Industrial Demonstration (ASTRID) (11) at End of Cycle (EOC), studied at KIT in the framework of the European Sustainable Nuclear Industrial Initiative (ESNII+).

The considered ASTRID core is a 1500 MW_{th} with two fuel zones (Fig. 4), including 177 and 114 fuel Sub-Assemblies, with different enrichment of the (U, Pu)O_2 fuel.

The core voided configuration is obtained removing the cooling sodium from all the fuel zones and from the intermediate fertile zone, the coolant in the inter-SA gaps being not removed.

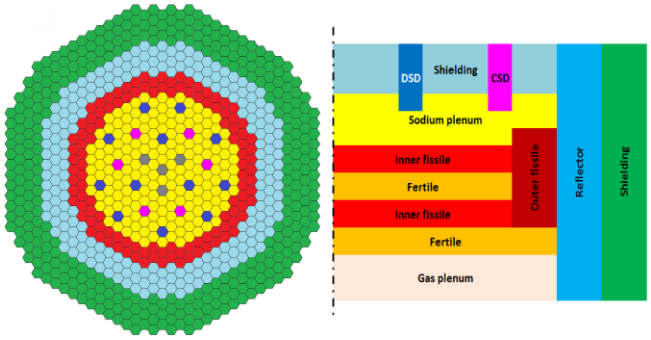

Fig. 4. ASTRID-like core map and vertical section at EOC, based on (11).

III. RESULTS

The results show that the employment of the GA in the SIMMER framework does make the code able to find a broad ES which can reproduce the reference structure. It is interesting analyzing the results shown in Fig. 5-7 and investigating the physical reasons that guide the evolution.

From Fig. 5 it is clear that a pattern associated with a good match of the k_{eff} with the objective one exists. The figure is particularly effective in showing the groups that should not be separated, namely the ones between ~20 keV and 500 eV; this energy range, as shown in Fig. 7, exactly corresponds with the largest resonance of sodium. Many other groups are formed around the resonances of the sodium (250-150 keV and 60-30 keV) or of the oxygen (1.3-0.8 MeV, 800-250 keV).

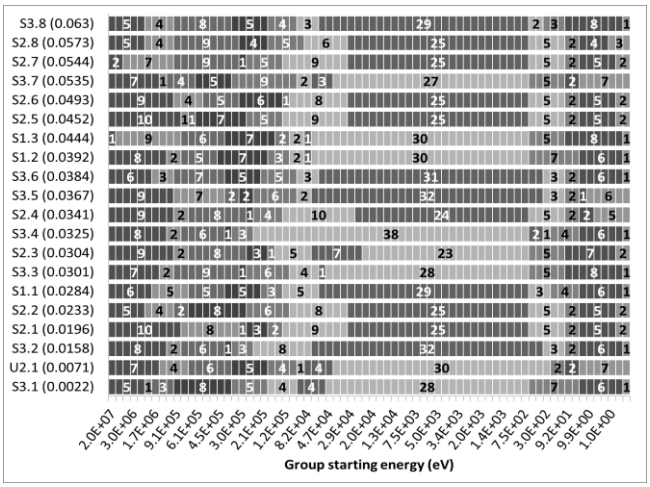

Fig. 5 Best found ESs associated with calculation ID and corresponding fitness.

Fig. 6 shows more clearly the tendency of the best solutions not to have energy cuts in the region of the main sodium resonance, and indicates the positions of some important energy cuts which are recurrent in most of the solutions (including the best one, Table I). The first one is placed between groups 9 and 10, at about 900 keV, and it represents a sort of boundary between the fast and the resonance spectrum zone, mainly related to the U^{238} fission XS; the other 4 cuts are all in the lower energy region, with the first one at 500 eV. The calculations show that these cuts, in particular the ones in the lower energy region, emerge in the first generations of the GA, and persist throughout the calculation; on the contrary, solutions not employing them succumb to selection and in-between alleles tend to extinction. One may suppose that they are just the results of the genetic drift without any physical meaning, also considering that the lower energy zone is not expected to be relevant for a fast reactor, but the fact that they appear in most of the calculation runs opposes to this hypothesis. Nevertheless, Fig. 6 and Fig. 7 show that energy cuts tend to concentrate in the energy regions where the neutron flux is high (between 300 keV and 2 MeV); this means that the ESs that invest more groups to describe zones with less neutrons are penalized in the selection process, i.e. they have worse fitness. As the energy cuts in the lower energy region look like an exception to this rule, they must be somehow useful to the energy space description. One possibility is that they are necessary to adequately represent the resonances in heavy nuclides XSs, like U^{238} and Pu^{239}, appearing in that energy range.

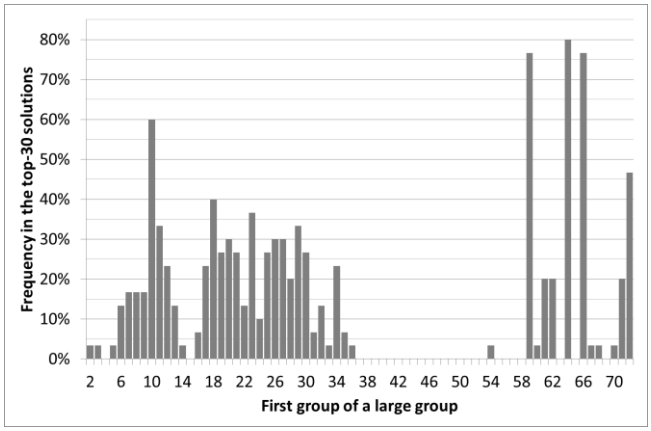

Fig. 6 Frequency of groups as new-groups starters in the top-30 solutions.

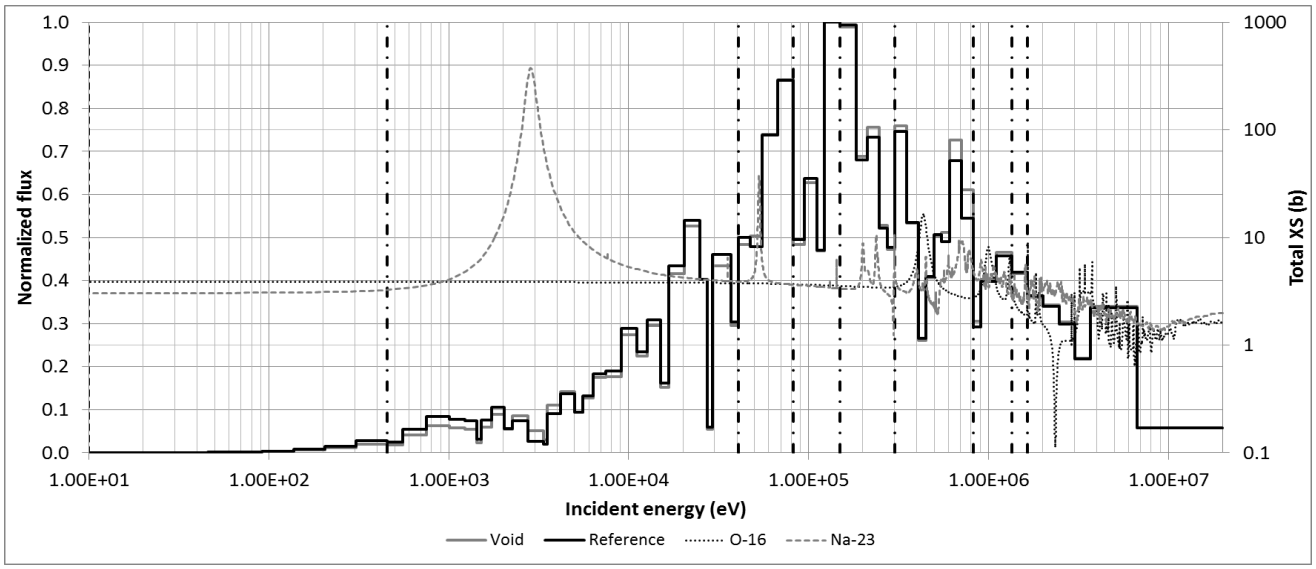

Fig. 7 ASTRID neutron spectrum in a fuel cell (in reference and voided conditions), relevant nuclides total XSs and best ES found.

Table I. Upper energy boundaries of the BL. Best estimated ES groups for the reference configurations are in bold.

Gr.	BL groups	Gr.	BL groups	Gr.	BL groups
1	**2.000E+07**	25	1.228E+05	49	3.355E+03
2	6.703E+06	26	1.111E+05	50	2.747E+03
3	3.679E+06	**27**	**9.482E+04**	51	2.249E+03
4	3.012E+06	28	8.230E+04	52	2.035E+03
5	2.466E+06	29	6.738E+04	53	1.722E+03
6	**2.019E+06**	30	5.517E+04	54	1.507E+03
7	**1.653E+06**	**31**	**4.748E+04**	55	1.434E+03
8	1.353E+06	32	4.087E+04	56	1.234E+03
9	1.108E+06	33	3.698E+04	57	1.010E+03
10	**9.072E+05**	34	2.928E+04	58	7.485E+02
11	8.209E+05	35	2.739E+04	**59**	**5.545E+02**
12	7.065E+05	36	2.479E+04	60	4.540E+02
13	6.081E+05	37	2.029E+04	61	3.043E+02
14	5.502E+05	38	1.662E+04	62	2.040E+02
15	4.979E+05	39	1.503E+04	63	1.367E+02
16	4.505E+05	40	1.273E+04	64	9.166E+01
17	4.076E+05	41	1.114E+04	65	4.552E+01
18	**3.508E+05**	42	9.119E+03	**66**	**1.945E+01**
19	3.020E+05	43	7.466E+03	67	9.906E+00
20	2.732E+05	44	6.320E+03	68	5.043E+00
21	2.472E+05	45	5.531E+03	69	2.130E+00
22	2.128E+05	46	5.005E+03	70	1.020E+00
23	**1.832E+05**	47	4.166E+03	71	4.850E-01
24	1.500E+05	48	3.527E+03	**72**	**1.890E-01**

1. Feedback coefficients

The feedback coefficients are key parameters for the reactor design; hence it is very important that the new ESs provide correct estimates of the k_{eff} also in conditions which are not those used for the GA run, so that the transient results are reliable at least until core degradation starts. For analyzing the next accidental phases, characterized by full core degradation, a new run of the GA may be necessary.

In order to verify this, the reference coefficients (i.e. calculated with all 72 available groups) are compared with the ones obtained using the GA best solution. As a further proof, the GA has been applied to the voided core, and the corresponding best solution has also been used to calculate the feedback coefficients. Table II summarizes the results.

Table II. Impact of ES on the feedback coefficients.

	FL	Best ES (Ref. conf.)	Best ES (Void conf.)
	k_{eff}		
Reference	0.99919	0.99920	0.99932
Voided core	1.00995	1.00980	1.00996
T_{fuel}+1000K	0.99633	0.99651	0.99669
	Feedback coefficients (pcm)		
Core void	+1066	+1051	+1054
K_D	-560	-527	-515

Both reference and voided-conditions solutions provide excellent results for both coolant void and Doppler feedback coefficients, with errors on the k_{eff} in the order of 20-30 pcm. The important values, i.e. the feedback coefficients, present even lower errors, acceptable for most applications.

This means that the reference conditions ES is not expected to lead to incorrect results in accidental conditions. However the small difference could be the effect of compensation among different energy groups.

2. Time performance

For the purpose of this study it is important to evaluate the time performances of both the genetic algorithm and SIMMER with the XS collapsing. Thus one can demonstrate that the time spent for the ES determination can be entirely covered by the corresponding reduction of the XS collapsing. The latter procedure can indeed be used without ES search, but this approach should be discouraged as results can be affected by large errors if the chosen ES is inappropriate.

The time performance measurement has been carried out using the Intel® VTune™ Amplifier 2015 profiler on a node with exclusive access of the InstitutsCluster II (IC2) (12), with processor Intel® Xeon® 5 (2.6 GHz).

A. CPU time required for the GA

In order to have uniform results, in each run the GA performs 6 generations with 50 individuals each. The measurement has been repeated 4 times for better results precision. Nevertheless, due to the stochastic choices intrinsic to the GA, the number of actual FF to be evaluated changes; in addition the fitness of any already examined individual is just retrieved from the storage tree, an operation which is much faster than the actual FF calculation. The results are shown in Table III and averaged in Table IV.

The final adjoint and real calculation, as expected, is longer than the doubled FF evaluation time as the flux acceleration described in §II.2.A is not applied.

Except for the time invested in objective k_{eff} calculation, which depends only on the FL, the other CPU time values are representative only if ESs with 11 groups are searched.

Table III. GA CPU time tests

	Test 1	Test 2	Test 3	Test 4
Individuals	300	300	300	300
FF calculations	262	249	250	259
Computational time per section (s)				
Total	1982.5	1945.9	1917.6	1951.2
Objective k_{eff}	58.0	57.8	58.0	56.4
Individuals FF	1899.2	1868.4	1837.3	1880.0
Final k_{eff} and k^+	24.6	19.1	21.7	14.2
SIMMER frame	0.7	0.6	0.6	0.6

Table IV. GA average CPU time results (s)

	Average	Corr. sample σ
Objective k_{eff}	57.5	0.8
FF calc. per individual	7.3	0.1
Final k_{eff} and k^+	19.9	4.4
SIMMER frame	0.6	0.03

B. XS collapsing time reduction

A 10 s stationary approach calculation of the ESNII+ core has been used for the estimation of the computational time of a SIMMER simulation. Both the actual CPU time and the neutronics/fluid-dynamics time share, of course, strongly depend on the model (number of thermal-hydraulic cells, neutronic mesh fineness, transient type, reactor state…). In order to reduce measurement uncertainty, calculations have been repeated 3 times for each considered number of groups, with 3 different ESs, in the same conditions described in previous paragraph.

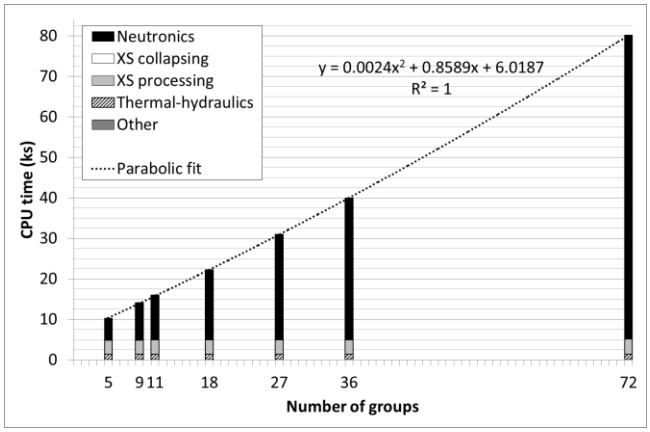

Fig. 8 CPU time for 10 s of stationary approach calculation with different number of groups using best estimated ESs.

Results in Fig. 8 show the CPU time dependence on the number of groups used: while thermal-hydraulics and XS processing time are not affected, the time required by the transport solver increases more than linearly with the number of groups. The time required by the XS collapsing procedure is almost negligible, being ~40 s in all cases, i.e. 0.4% of the total CPU time at most (72→5 groups). The XS processing time is constant, as this procedure is performed on the FL, which has 72 groups in all considered cases.

C. GA convergence speed

Estimating the number of individuals to be examined before convergence to a reasonable ES is not an easy task: it requires sensitivity studies on all different GA parameters, such as initial population size, growth rate, mutation rate, selection pressure. Such tests would allow estimating the minimum number of individuals that, on average, are needed for convergence. These optimization studies are considered of interest for the future, along with the evolution of the GA to an Adaptive Genetic Algorithm (13), which would improve the convergence rate.

A preliminary estimate of the number of individuals required for the 72→11 groups collapsing problem has anyhow been done. The GA has been run with 3 different

population sizes (twice each), keeping the selection pressure constant (5 individuals per tournament on average). The termination criterion is the achievement of a fitness value lower than 1, i.e a discrepancy on the multiplication factor in the order of 1 pcm; such difference is considered acceptable for most types of calculation.

Table V. GA average CPU time results (s)

Initial population	50	100	150
Growth rate	1.0	1.0	1.0
Mutation rate	5%	5%	5%
Elitism rate	2%	2%	2%
Number of tournaments	10	20	30
Tournament parameter *p*	0.1	0.1	0.1
Number of generations	16	39	20
	40	35	18
Considered individuals	800	3900	3000
	2000	3500	2700
Unique individuals	650	3106	2715
	1553	2985	2434

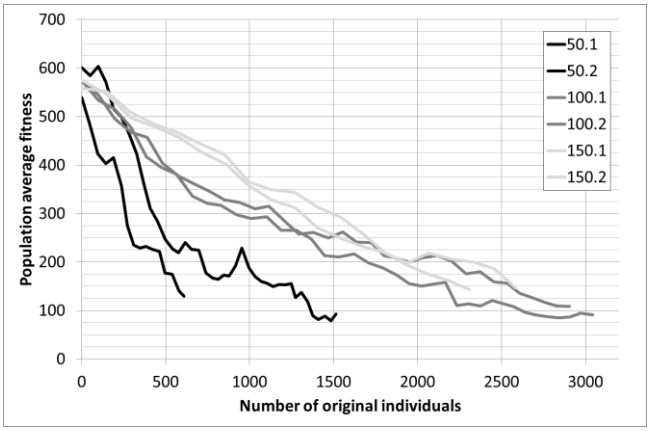

Fig. 9 Population average fitness convergence speed.

The results summarized in Table V suggest that a smaller initial population converges faster to the solution; anyhow Fig. 9 shows that the convergence of such populations is more erratic, being more susceptible to initial random sampling and genetic drift. Also, a faster convergence of the population average fit might not be an advantage, as the lower genetic variability would affect the exploration capability of the population, which could end up prematurely converging toward a local optimum. The convergence speed point should be studied more in depth, but the performed calculations provide a preliminary average number of unique individuals required to achieve convergence, being for the present case 2241±956.

Based on results shown in Fig. 8, a calculation with 11 energy groups would reduce the computational time with respect to the 72 groups BL case by 64 ks (80%) for the first 10 s of simulation. Combining this result with Table IV data, the same computational time can be used to take into consideration more than 8500 unique solutions, more than double of the required estimate increased by 2σ.

Moreover, the ES has to be calculated only once for each reactor system but can be used for different simulations, provided that the reactor conditions do not change excessively. Finally, the CPU time reduction has been calculated for 10 s of simulations, but much longer time spans (at least a few minutes of simulation) have to be considered when performing safety studies, making the time reduction in absolute terms extremely favorable.

IV. CONCLUSIONS

An automated tool aiming to the energy meshing selection for multigroup XS libraries has been presented. The procedure is based on a genetic algorithm and is coupled with the safety analysis code SIMMER. The tests performed on the ESNII+ ASTRID-like reactor system show that the GA is able to suggest energy structures for the considered problem which correctly predict the multiplication factor both in reference and out-of-nominal conditions.

The problem constraints have been established and a non-binary chromosome representation able to respect them has been devised. The genetic operators have been chosen in order to respect the problem boundaries and to leave the user the freedom of both choosing the number of groups in the solution and easily tuning the GA parameters.

The fitness function, i.e. the measure of the studied solution "goodness", is based on the difference between the k_{eff} obtained with the considered ES and the objective one, calculated at the start of the GA with the FL. The fitness calculations are the operations employing most of the computational time, so the procedure has been accelerated using a binary tree, where new fitness are stored as they are calculated to be retrieved in case they are needed again, and by collapsing the flux calculated with the FL, which provides an educated guess to the transport solver and so faster convergence.

The tests focus on the search of an 11-groups energy structure for the collapsing of the 72-groups fine-library. The energy structure determined by the GA adequately model the reactor in reference conditions, so demonstrating the effectiveness of the approach in the problem solution. The GA has also been applied to the reactor in out-of-nominal conditions; the study is of interest to predict the effect of the ES on accidental transient simulations. The results show that the discrepancies of the feedback coefficients are acceptable in all considered cases, both when the ES is calculated with the reactor in its reference state and when a voided configuration is used.

The computational time in a selected 10 s transient is dominated by the transport solver, so it can be strongly reduced by using XS libraries with less energy groups; results show that the link between CPU time and number of energy groups is quadratic. Based on the parabolic fit, XS

collapsing from 72 to 11 energy groups is able to reduce the CPU time by 80%. This, considering that accidental transient SIMMER calculations can take days or even weeks, makes the XS collapsing an extremely powerful tool, if one is able to use the correct energy structure. The GA cares for this last point.

Preliminary results suggest that on average 2241 individuals have to be examined before the discrepancy on the multiplication factor is reduced to the order of 1 pcm, acceptable for most applications. Considering that the fitness function evaluation takes 7.3 s per individual, the GA would converge within just a small fraction of the spared time; moreover one should consider that the energy structure can be used for all simulations related to the reactor, provided that the initial conditions do not change too much.

Finally, the convergence speed can be improved by optimization of the parameters and by passing to Adaptive Genetic Algorithm, both activities considered of interest for future studies. Also, the methodology can be further improved by implementing other fitness functions, possibly taking into account the reaction rates and the neutron flux, which effect, as shown, plays a relevant role on the energy structure definition.

NOMENCLATURE

C = individual chromosome
FG = number of groups in the coarse ES
f_I = fitness associated to individual I
g = generic group of the FL
G = generic group of the BL
MG = number of groups in the fine ES
R_I = ranking of individual I in its tournament

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