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UNSTRUCTURED 3D CORE CALCULATIONS WITH THE DESCARTES SYSTEM APPLICATION TO THE JHR RESEARCH REACTOR

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ABSTRACT

Recent developments in the DESCARTES system enable neutronics calculations dealing with very complex unstructured geometrical configurations. The discretization can be made either by using a very fine Cartesian mesh and the fast simplified transport (SPN) solver MINOS, or a discretization based on triangles and the SP1 solver MINARET. In order to perform parallel calculations dealing with a very fine mesh in 3D, a domain decomposition with non overlapping domains has been implemented. To illustrate these capabilities, we present an application on the future European research reactor JHR dedicated to technological irradiations.

Key Words: Neutronics, Finite Elements, Parallelization, Unstructured geometry

1. INTRODUCTION

A new generation reactor computational system, named DESCARTES, has been elaborated in cooperation of CEA, AREVA/NP and EDF [1]. The main goal of the architecture design of DESCARTES is to provide a complete tool for neutronics calculations based on a set of operators acting on shared objects. This toolbox has to perform neutronics calculations for various reactor types, from industrial applications to reference calculations, and to permit R&D in numerics and physical modeling.
Recent developments in the DESCARTES system make it possible to compute solutions dealing with very complex unstructured geometrical configurations by using the fast simplified transport (SPN) solver MINOS on a very fine Cartesian spatial mesh or the SP1 solver MINARET using arbitrary triangles as discretization. A mesh generator, which preserves the physical volumes of the geometry, has been developed for this purpose.
To illustrate these capabilities, we present an application on the future European research reactor, the Jules-Horowitz-Reactor (JHR) [2], dedicated to technological irradiations.

2. THE DESCARTES DATA MODEL

The main part of the DESCARTES architecture resides on an internal data model (IDM), which gives the possibility to define objects shared by the different components (for example, the different solvers). Among these shared elements, the geometrical object describes the geometry of the core and its material constitution. The geometrical component allows the user to describe highly heterogeneous geometrical structures using a hierarchical description. Other shared elements describe the parametric microscopic cross sections associated to the different materials and macroscopic cross sections for the different regions of the core.
The other part of the architecture lies on a set of operators or solvers, which work on the shared objects of the IDM. The main core solver for Cartesian geometry, named MINOS [3], provides fast calculations with low memory requirements, making it possible to carry out calculations on very fine meshes. Moreover, another new solver MINARET makes possible calculations based on a triangulation of the core.

3. THE GEOMETRICAL CORE COMPONENTS

The geometrical component is used to describe the distribution of the different materials within the core. As the geometrical elements composing the core are often obtained by repetition, the geometrical data are given in a hierarchical form. Each level of the hierarchy represents a flat component that can be either represented by a combination of elementary volumes, by a collection of volumes defined by their surface boundaries or by regular meshes (Cartesian or hexagonal). For a standard core calculation, the representation of the geometry is usually composed of 3 levels. The first one describes the radial distribution of the fuel assemblies and of the reflectors in the core; the two other levels give respectively the description of the axial and radial composition of each assembly.
For the acquisition of the complex geometries, an interface makes it possible to read geometries built with the graphical user interface SILENE developed at CEA [4]. In the SILENE software, the geometry is described by a collection of objects representing nodes (points), equations (segments of straight lines, circles, arcs of circles and arcs of involutes of circles), meshes, axial levels (3D), and distribution of the materials.
These different objects are then treated in the geometrical interface of DESCARTES in order to generate the set of regions (domain) defined by their surface edges and also their neighboring regions. Each region is supposed to be homogeneous and composed by one material.
In order to perform the flux calculation using the Cartesian solver MINOS, the complex geometry has to be projected on a very fine Cartesian grid. This projection generates heterogeneous volumes that are taken into account in the MINOS solver by an homogenization technique which preserves the volumes of the different media.
In the case of a small reactor configuration as for research reactor a 1000x1000x30 mesh is sufficient.
Another way consists in a discretization of the different regions of the geometry into a collection of triangles; a specific geometrical component generates automatically a triangulation of the different physical regions of the core domain.
The mesh generation is done in several steps. First for each physical region of the geometry, a surface mesh is defined to approximate the border of the region. The positions of the border points of the triangulation are automatically settled in order to preserve the volume of the

physical regions. The surface mesh size can vary according to its position in the core. The second step consists in the generation of a set of points inside the physical region. The inner points are uniformly set out in order that the distances between two neighboring points are close to the average distance between the surface points. Then, a triangulation is generated by tessellation of the previous point distribution using a Delaunay algorithm. The final step consists in a smoothing algorithm, which recalculates the distribution of the internal points by a harmonic transformation in order to improve the quality of the triangle (maximization of the minimal angle). The hierarchical structure of the geometry is kept in order to perform in the future, multigrid acceleration and parallel calculations. Figure 1 shows as example, the distribution of the original physical regions in a part of the JHR core (on the left side) and the generated mesh obtained by the previous algorithm (on the right side).

4. THE MINOS SOLVER

The MINOS solver has been used for several years as core calculation tool in the SAPHYR system [5]. The MINOS solver (initially written in F77) has been rewritten within the DESCARTES context by using an object oriented design and C++ programming language. The numerical method of the original solver was kept, but its general architecture was reconsidered in order to improve its capability of evolution and its maintainability. Moreover, the performances of the older version have been improved.
MINOS solves the SPN approximation to the transport equation on a Cartesian geometry. It is based on the mixed dual finite element approximation of the simplified transport equation (SPN) The Raviart-Thomas-Nedelec elements[8] (RTN) are used to discretize the different functional spaces. For very fine mesh calculations, low order approximation and numerical integration are used (RT0).
The iterative algorithm used to solve the within-group source equations can be viewed as an alternating direction sweep, performed on the different components of the current vector.

5. THE MINARET SOLVER

MINARET is a new solver recently implemented in the context of the DESCARTES platform. As the MINOS solver, it is based on object oriented design and C++ programming language. This solver is aimed to treat 3D complex cylindrical geometries using an unstructured radial mesh composed by triangles of any shape.
An SP1 solver has been implemented taking into account the triangular mesh described in section 3, it uses the mixed dual formulation of the SP1 equations (the same as in MINOS). The discretization is based on the Raviart-Thomas finite element on the triangle (RT0) [8]. With this approximation, the flux is supposed to be constant within each triangle, and the current is approximated with a linear polynomial basis. The iterative algorithm consists first in the elimination of the flux unknowns and then to get a linear system having as unknowns the normal current on each edge of the triangulation. The linear source problem is then solved using a preconditioned conjugate gradient by a SSOR preconditionner.

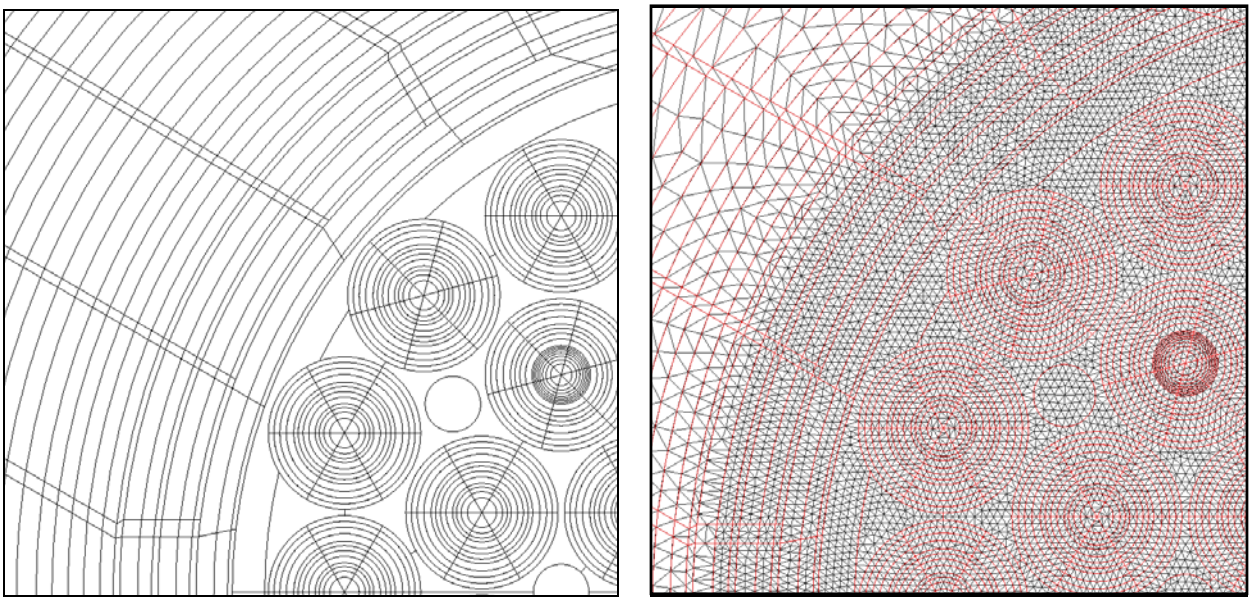

Figure 1. Part of the physical domain and its discretization by a triangular mesh

6. PARALLEL PROCESSING

In order to use parallel computers, an iterative domain decomposition method (IDD)[6][9] has recently been implemented in the MINOS solver. This method is an iterative scheme, using non-overlapping domain decomposition and is based on the exchange of boundary values. The idea is to iterate the resolution of local problems on each subdomain, using Robin interface conditions. This condition at a given iteration consists in imposing the corresponding boundary value of the solution obtained on the adjacent subdomain at the previous iteration.
The main advantage of the IDD method is that it needs only minor modification of the MINOS solver. Only two data exchanges per outer iteration are necessary between the processes: one for the interface condition exchange between the adjacent subdomains, and one for the eigenvalue calculation. The domain decomposition is automatic, by imposing the same size for all the subdomains, and ensures a good balance of the load of the processors. This method is highly and easily parallelizable, and well-fitted for heterogeneous core calculations. This method is general and can be easily extended to other solvers. In the future it will be interfaced with MINARET.
In Fig. 2, we present a domain decomposition in 16 subdomains for the JHR core.

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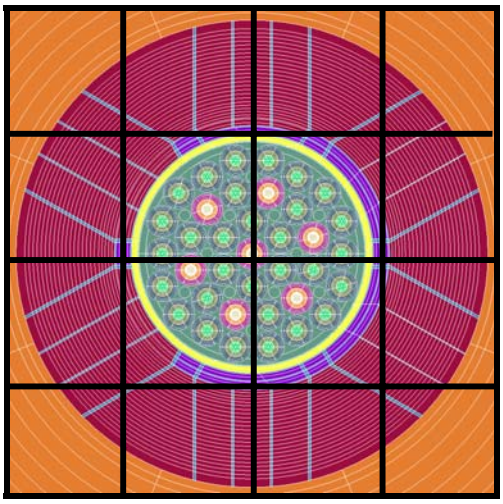

Figure 2. Decomposition in 16 subdomains for the JHR core.

7. THE NUMERICAL APPLICATION

To illustrate the previous methodologies, we have performed a first 2D calculation corresponding to a starting configuration for the JHR research reactor core. The core is composed of 37 fuel assemblies (arranged in 4 rings). Each assembly is composed by 3 groups of 8 cylindrical fuel plates, maintained by three aluminum stiffeners. The core is surrounded by a beryllium reflector and a water reactor pool. For our applications, seven assemblies contain an absorbing medium (Hafnium). All calculations are performed with a 6 energy group data library and 13 different materials. In all the calculations the scattering cross sections are of angular order P1. The results are compared with those obtained by Monte Carlo calculations with the Tripoli4 code and a point wise description of the cross sections [7]. It should be noted that the high value of Keff is due to the fact that the axial buckling is not taken into account and also that the core corresponds to the beginning of cycle.
Figure 3 presents three different levels of geometry, starting from the input geometry given by the SILENE GUI, consisting of 4471 nodes, 8737 edges and 4287 physical regions. The second geometry is the material geometry of DESCARTES, the third one is the projection of the previous geometry on a 1000x1000 grid which is used by the MINOS solver.

The three first results concern the MINOS calculations.
Table I has been obtained with MINOS for a 2D configuration and a 1000x1000 grid on three different computer platforms. In Table II, the calculations are carried out with three different mesh refinements (1000x1000, 2000x2000 and 3000x3000 discretization), representing respectively 18M, 72M and 162M of unknowns. The relative flux precision is 10^{-3}. Finally, Table III gives the results with a 1000x1000 grid refinement and different number of harmonics for the angular approximation. The results show that the calculation is much more sensitive to the angular approximation than for the spatial refinement. The results are very close to the reference calculation given by a Tripoli4 reference transport calculation.
Table IV gives the results obtained with the MINARET solver. The first calculation (first line) corresponds to a mesh where the size of the triangles is constant inside the active part of the core and increases until the periphery (from 0.4cm to 1cm). The next line of the table presents a

calculation using a mesh obtained from the previous by splitting each triangle into 4 triangles. The last line gives the results for a mesh obtained by splitting a second time. The results are close to the one obtained with MINOS.
Table V shows the efficiency of domain decomposition method on a parallel computer. The calculation given in the first line of the table corresponds to the standard MINOS calculation with a 1000x1000 grid. The other results have been obtained by varying the number of subdomains and processors (one by subdomain). As shown we get an important decrease of the computing time with an efficiency greater than 1, due to a best utilization of the cache memory.
The last table (Table VI) concerns the very first 3D calculation performed with a grid discretization of 1000x1000x28 mesh and the MINOS solver for the sequential version and also with parallel calculation. The computing time is close to be proportional to the number of mesh points with respect to 2D calculations.
Finally, Fig. 4 presents the power map calculated by the MINOS solver and Fig. 5 presents the flux distribution for the 6 energy groups obtained with a 1000x1000 grid mesh.

Table I. 2D MINOS calculation on different computer plateform (Reference transport calculation Tripoli4 : Keff=1.31239), flux precision=10-3

Processor	Mesh	Approx	Keff	Power peak	CPU time (s)	Number of iterations
Intel Xeon 3.6 GHz 4Gb Ram	1000x1000	SP1	1.30714	2.68	364	334
AMD Opteron 2,6 GHz 32Gb Ram	1000x1000	SP1	1.30718	2.67	365	338
HP ES80 EV7 1.15 GHz 32Gb Ram	1000x1000	SP1	1.30718	2.67	380	338

Table II. 2D MINOS calculation for different grid refinements Reference calculation Tripoli4 : Keff=1.31239, prec=10-3 on AMD Opteron 2,6 GHz)

Mesh	Approx	Keff	Power peak	CPU time (s)	Number of iterations
1000x1000	SP1	1.30718	2.67	365	338
2000x2000	SP1	1.30691	2.70	1297	285
3000x3000	SP1	1.30704	2.70	3071	291

Table III. 2D MINOS calculation for different SPN order, 800 outer iteration and a 1000x1000 grid, AMD Opteron 2,6 GHz

Approx	Keff	Power peak	CPU time (s)
SP1	1.30739	2.656	1021
SP3	1.31334	2.627	2251
SP5	1.31391	2.582	2937
SP7	1.31415	2.577	4370

Table IV. 2D MINARET SP1 calculation for different triangle size on AMD Opteron 2,6 GHz

Mesh (nb of triangles)	Mesh (nb of edges)	Keff	Power peak by physical regions	CPU time (s)	Number of iterations
82373	124332	1.30717	2.314	261	26*470
325991	497280	1.30681	2.326	2117	40*750
1303976	1989024	1.30757	2.329	8657	40*860

Table V. Results for the parallel processing of the 2D JHR, comparison with a full converged MINOS calculation with 50 000 outer iterations. $k_{eff} = 1.30857$ **.**

Number of processors	**Number of outer iterations**	Δk_{eff} (pcm)	**Elapsed time (s.)**	**Efficiency per iteration (%)**
Sequential	941	78	1490	100
2	917	78	581	125
4	978	78	357	108
8	950	64	165	114
16	978	55	76	127
25	1129	52	55	130
36	1062	58	34	138

Table VI. JHR 3D 1000x1000x28 grid, MINOS SP1 calculation with 1000 outer iterations Keff=1.13938

Number of processors	Elapsed time (s.)	Efficiency per iteration (%)
Sequential	63613	100
4	20832	76
6	15513	68

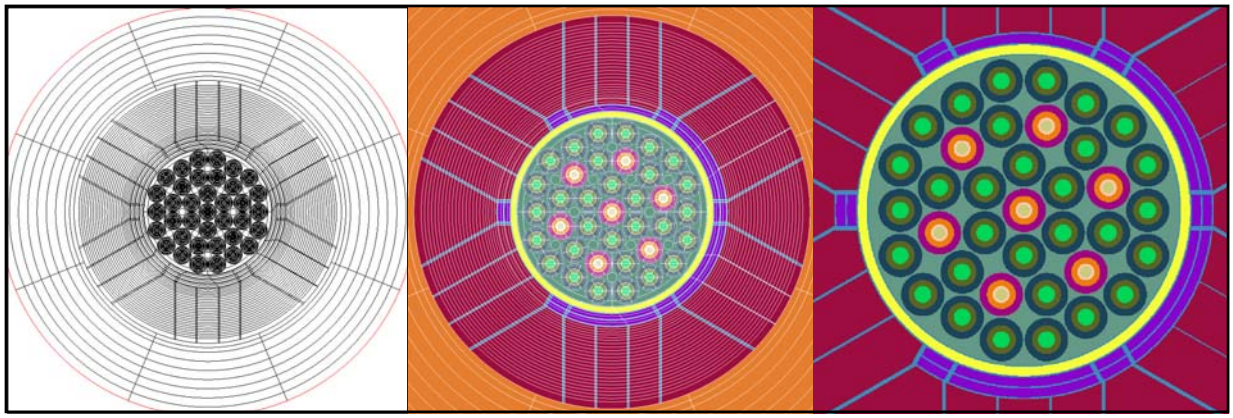

Figure 3. The three different levels of geometrical representation

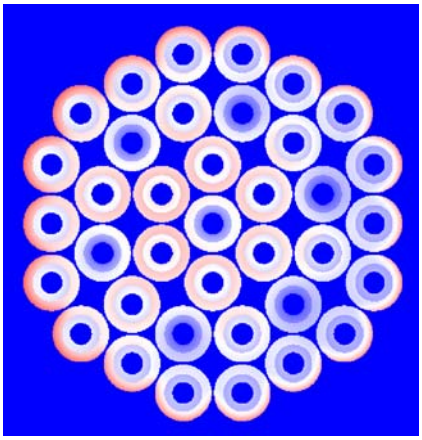

Figure 4. The power map

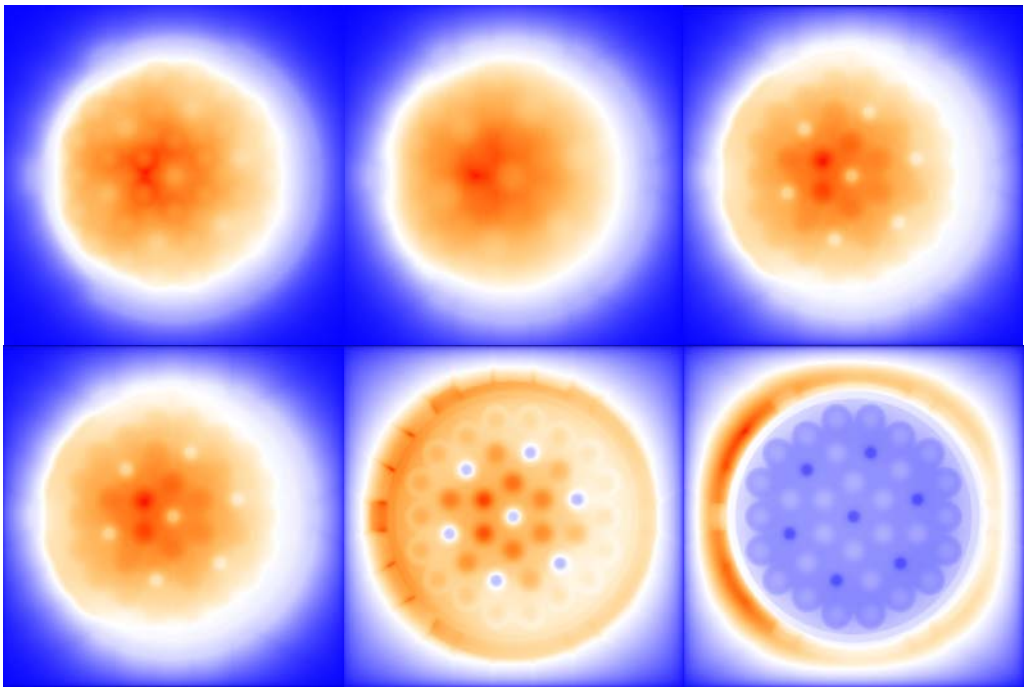

Figure 5. The flux distribution for the 6 energy groups

8. CONCLUSION

This paper presents the new possibilities that are now available within the DESCARTES system. These calculations are made possible thanks to the availability of three powerful tools: first the SILENE graphical user interface, which allows the user to devise graphically very complex 3D geometries; then, the flexible internal data model of DESCARTES which allows to take into account these complex geometries; finally, the MINOS and MINARET solvers which perform core calculations on a very fine grid. To illustrate these capabilities, we performed a 3D calculation on the future research reactor JHR.

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