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A MULTI-SCALE APPROACH FOR THE NEUTRONIC KINETICS EQUATIONS USING THE MIXED DUAL SOLVER MINOS

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ABSTRACT

In order to improve the time/precision ratio of the simulation calculations, we investigate a multi-scale technique for the resolution of the reactor kinetics equations. We choose to focus on the mixed dual diffusion approximation and the Quasi-Static method. We introduce a space dependency for the amplitude function which only depends on the time variable in the standard Quasi-Static context. With this new factorization, we develop two mixed dual problems which can be solved with CEA's solver MINOS. An algorithm is implemented, performing the resolution of these problems defined on different scales (for time and space). We name this approach the Local Quasi-Static method. The consistency of the model and the pertinence of our first modeling and discretization choices are studied for a simplified test. The first results are incomplete but satisfactory. Furthermore, they open new possibilities on parallelization and adaptive scales.

Key Words: Neutronic, Kinetics, Diffusion, Quasi-Static, Multi-Scale

1. INTRODUCTION

Within the context of the reactor core simulations, we consider the resolution of the neutronic kinetic equations with the diffusion approximation. The Improved Quasi-Static method (IQS) [7] is based on a factorization of the neutronic flux ϕ, solution of these equations, distinguishing an amplitude function a, constant in space, and a shape flux f which depends weakly on the time variable. The hypothesis on the amplitude imposes to frequently update the shape in order to take into account the space variations. For accurate simulation, the IQS method, which has been implemented [2, 3] in CRONOS code [9], is not really better, for the time/precision ratio, than the direct resolution of the diffusion equations. For this reason, we develop a multi-scale approach, named Local Quasi-Static (LQS). We introduce a coarse space dependence for the amplitude function, as the IQS method has introduced a shape coarse time variation, compared with first Quasi-Static method.

The resulting reformulated problem is presented in the following section. Then, in the third part, we investigate the space and time discretizations, our hypothesis on the time variation and a normalization condition, which makes the factorization unique. Some details of our implementation and the resulting

algorithm are discussed in the section four. Finally, the last section contains our first numerical results for simplified cases, illustrating consistency and convergence.

2. MIXED FORMULATION OF LOCAL QUASI-STATIC PROBLEM

This section is subdivided in two parts. First, the LQS formulation is explained. Then, the choices of this new formulation are briefly discussed.

2.1. Mixed Dual Equations and Factorization

For the following problems, the mixed dual formulation has been preferred in order to be able to use the optimized solver MINOS which is available in the framework of the CRONOS system [1]. The system of equations studied here comes from the multigroup kinetics diffusion equation in mixed formulation :

$$\left\{\begin{array}{l} \dfrac{1}{V^g}\dfrac{\partial \phi^g}{\partial t} = -\overrightarrow{\nabla}.\overrightarrow{p_\phi^g} - \displaystyle\sum_{g'}\left(\Sigma_t^g - \chi_p^g(1-\beta^{g'})\nu\Sigma_f^{g'} - \Sigma_s^{g'g}\right)\phi^{g'} + \sum_{k=1}^{K}\chi_d^{kg}\lambda^k c^k\,, \\ \overrightarrow{p_\phi^g} = -D^g\overrightarrow{\nabla\phi^g}\,, \\ \dfrac{\partial c^k}{\partial t} = -\lambda^k c^k + \displaystyle\sum_{g'}(\beta\nu\Sigma_f)^{kg'}\phi^{g'}\,, \\ \phi^g_{|\Gamma_D} = 0\,,\ (\overrightarrow{p_\phi^g}.\overrightarrow{n})_{|\Gamma_N} = 0\,,\ (\overrightarrow{p_\phi^g}.\overrightarrow{n})_{|\Gamma_R} = \displaystyle\sum_{g'}(\tau)^{gg'}\phi^{g'}, \end{array}\right. \tag{1}$$

with usual notations :

- ϕ^g is the neutronic flux for the energy group g;
- $\overrightarrow{p_\phi^g}$ is the current vector associated to the flux for the group g;
- V^g is the neutrons speed for the group g;
- D^g is the diffusion coefficient for the group g;
- Σ_t^g is the total cross section for the group g;
- Σ_f^g is the fission cross section for the group g;
- $\Sigma_s^{g'g}$ is the scattering cross section from the group g' to the group g;
- χ_p^g and χ_d^{kg} are the spectra of the prompt and delayed neutrons for the group g;
- β^{kg} is the fraction of delayed neutrons of the precursor group k and β^g the total for the group g ($\beta^g = \sum_{k=1}^{K}\beta^{kg}$);
- ν is the fission ratio;
- λ^k is the decay constant of delayed neutron in group k;
- c^k is the precursor concentration of the group k.

For our resolution method, we introduce a total production cross section from the group g' to the group g :

$$\chi^g \nu\Sigma_f^{g'} = \chi_p^g(1-\beta^{g'})\nu\Sigma_f^{g'} + \sum_{k=1}^{K} \chi_d^{kg}\beta^{kg'}\nu\Sigma_f^{g'} .$$

So, we obtain the following problem to solve :

$$\left\{ \begin{array}{l} \dfrac{1}{V^g}\dfrac{\partial\phi^g}{\partial t} = -\overrightarrow{\nabla}.\overrightarrow{p_\phi^g} - \displaystyle\sum_{g'}\left(\Sigma_t^g - \chi^g\nu\Sigma_f^{g'} - \Sigma_s^{g'g}\right)\phi^{g'} + S_d^g \,, \\ \overrightarrow{p_\phi^g} = -D^g\overrightarrow{\nabla\phi^g} \,,\ S_d^g = -\displaystyle\sum_k \chi_d^{kg}\frac{\partial c^k}{\partial t} \,, \\ \dfrac{\partial c^k}{\partial t} = -\lambda^k c^k + \displaystyle\sum_{g'}(\beta\nu\Sigma_f)^{kg'}\phi^{g'} \,, \\ \phi^g_{|\Gamma_D} = 0 \,,\ (\overrightarrow{p_\phi^g}.\overrightarrow{n})_{|\Gamma_N} = 0 \,,\ (\overrightarrow{p_\phi^g}.\overrightarrow{n})_{|\Gamma_R} = \sum_{g'}(\tau)^{gg'}\phi^{g'} . \end{array} \right. \tag{2}$$

Then, we introduce the quasi-static factorization :

$$\phi^g(\overrightarrow{r},t) = a^g(\overrightarrow{r},t)f^g(\overrightarrow{r},t) \tag{3}$$

where a is the amplitude function and f is the shape flux. From this factorization and Fick's law, we deduce a decomposition of the current which results from the definitions of the currents associated to the amplitude a and the shape f :

$$\overrightarrow{p_\phi} = -Df\overrightarrow{\nabla a} - Da\overrightarrow{\nabla f} = \overrightarrow{p_a} + \overrightarrow{p_f} \,. \tag{4}$$

When one solves a mixed dual problem, the normal traces of the current are continuous (by definition of the space discretization) and the definition (4) implies that the reconstructed current has the same property.

2.2. Two Different Problems

After some manipulations, two symmetric problems are obtained : one for the amplitude function a, supposing that f is known :

$$\left\{ \begin{array}{l} \dfrac{f^g}{V^g}\dfrac{\partial a^g}{\partial t} = -\overrightarrow{\nabla}.\overrightarrow{p_a^g} - \displaystyle\sum_{g'}\left(\Sigma_t^g - \chi^g\nu\Sigma_f^{g'} - \Sigma_s^{g'g}\right)f^{g'}a^{g'} - \frac{1}{V^g}\frac{\partial f^g}{\partial t}a^g + S_e^g(c^k,f^g) \,, \\ \overrightarrow{p_a^g} = -D^g f^g\overrightarrow{\nabla a^g} \,, S_e^g(c^k,f^g) = -\displaystyle\sum_k \chi_d^{kg}\frac{\partial c^k}{\partial t} - \overrightarrow{\nabla}.\overrightarrow{p_f^g} \,, \\ \dfrac{\partial c^k}{\partial t} = -\lambda^k c^k + \displaystyle\sum_{g'}(\beta\nu\Sigma_f)^{kg'}f^{g'}a^{g'} \,, \\ (\overrightarrow{p_a^g}.\overrightarrow{n})_{|\Gamma_D\cup\Gamma_N\cup\Gamma_R} = 0 \end{array} \right. \tag{5}$$

and one for the shape flux f, supposing that a is known :

$$\left\{\begin{array}{l} \dfrac{a^g}{V^g}\dfrac{\partial f^g}{\partial t} = -\overrightarrow{\nabla}.\overrightarrow{p_f^g} - \displaystyle\sum_{g'}\left(\Sigma_t^g - \chi^g\nu\Sigma_f^{g'} - \Sigma_s^{g'g}\right)a^{g'}f^{g'} - \dfrac{1}{V^g}\dfrac{\partial a^g}{\partial t}f^g + S_e^g(c^k,a^g)\,, \\ \overrightarrow{p_f^g} = -D^g a^g\overrightarrow{\nabla f^g}\,, S_e^g(c^k,a^g) = -\displaystyle\sum_k \chi_d^{kg}\dfrac{\partial c^k}{\partial t} - \overrightarrow{\nabla}.\overrightarrow{p_a^g}\,, \\ \dfrac{\partial c^k}{\partial t} = -\lambda^k c^k + \displaystyle\sum_{g'}(\beta\nu\Sigma_f)^{kg'}a^{g'}f^{g'}\,, \\ f^g_{|\Gamma_D} = 0\,,\ (\overrightarrow{p_f^g}.\overrightarrow{n})_{|\Gamma_N} = 0\,,\ (\overrightarrow{p_f^g}.\overrightarrow{n})_{|\Gamma_R} = \sum_{g'}(\tau)^{gg'}a^{g'}f^{g'}\,. \end{array}\right. \tag{6}$$

To guarantee the unicity of the decomposition (3) and to simplify the time derivative of f in problem (5), as in standard quasi-static method, a normalization condition is presented in the following section. For these problems, we suppose the existence and the unicity of the solutions. Then, their respective solutions must be strictly positive inside the domain Ω. If the physical consistency imposes it, mathematically, the result is more difficult to obtain. Some demonstrations of the literature [4, 5] give us the first properties. But, the strict positivity remains to study.

Compared to IQS method, the amplitude problem is more complex. In fact, the equations (5) are discretized and solved for a coarse scale in space but a fine scale in time. It is the opposite for the shape. In a more global point of view, the solution reconstructed with equation (3) and the solutions of problems (5) and (6) satisfy the boundary conditions and the system of equations (2). We expect that an amplitude which depends coarsely of the space variable should better take into account the heterogeneity of the geometric and neutronic data.

We have chosen to keep a mixed dual formulation for both problems because our solver is based on this formulation. Moreover, this symmetric reformulation enables to have a reconstructed solution which have the same properties (discontinuous flux and continuous current) than one obtained with a reference solver. Nevertheless, nothing in this modeling imposes a specific solver. A priori, the LQS method can be adapted to all the diffusion solvers.

3. DISCRETIZATIONS AND RESOLUTIONS

As there are two different problems, there are two different strategies of discretization which are discussed in this section.

3.1. Amplitude Calculation

In space, we dicretize the amplitude and its current with a coarse Raviart-Thomas basis [8]. So, we can consider that the equations (5) are condensed on a set of disjointed subdomains $(\Omega_s)_{i=1,..S}$ which are the meshes of the finite elements method. In the following equations, we use :

$$\left\{\left(B_i^{(0)}\psi_0\right)_{i=1,..N}, \left(\left(B_{j_d}^{(1,d)}\right)_{j_d=1,..,M_d}\right)_{d=x,y,z}\right\} \tag{7}$$

where $B_i^{(0)}$ is a basis function for the flux, $B_{j_d}^{(1,d)}$ is a basis function for the current in d direction and ψ_0 is an inserted weight function constant in time. After projection, a weak formulation of equations (5) reads

for the function :

$$\begin{aligned}\sum_{i=1}^{N}\frac{\partial a_i}{\partial t}\int_\Omega V^{-1}f\psi_0^2B_i^{(0)}B_{i'}^{(0)}\overrightarrow{dr} = &-\sum_{d=x,y,z}\sum_{j_d=1}^{M_d}p_{a,d,j_d}\int_\Omega\frac{\partial B_{j_d}^{(1,d)}}{\partial d}\psi_0B_{i'}^{(0)}\overrightarrow{dr}\\ &-\sum_{i=1}^{N}a_i\int_\Omega\left(\Sigma_t-\chi\nu\Sigma_f-\Sigma_s\right)f\psi_0^2B_i^{(0)}B_{i'}^{(0)}\overrightarrow{dr}\\ &-\sum_{i=1}^{N}a_i\int_\Omega V^{-1}\frac{\partial f}{\partial t}\psi_0^2B_i^{(0)}B_{i'}^{(0)}\overrightarrow{dr}\\ &+\int_\Omega S_e(c,f)\psi_0B_{i'}^{(0)}\overrightarrow{dr}\,,\end{aligned}\tag{8}$$

for its associated current :

$$\sum_{j_d=1}^{M_d}p_{a,d,j_d}\int_\Omega(fD)^{-1}B_j^{(1,d)}B_{j'_d}^{(1,d)}\overrightarrow{dr}-\sum_{i=1}^{N}a_i\int_\Omega\frac{\partial B_{j_d}^{(1,d)}}{\partial d}\psi_0B_{i'}^{(0)}\overrightarrow{dr}=0\tag{9}$$

and for the precursor concentration :

$$\int_\Omega\frac{\partial c}{\partial t}\chi_d\psi_0B_{i'}^{(0)}\overrightarrow{dr}=-\lambda\int_\Omega c\chi_d\psi_0B_{i'}^{(0)}\overrightarrow{dr}+\int_\Omega\beta\nu\Sigma_f af\chi_d\psi_0B_{i'}^{(0)}\overrightarrow{dr}\,,\tag{10}$$

with a simplified notation omitting the group indices. Thus, a condensed system is obtained with the local values of the amplitude as unknowns.

The LQS method can be viewed as an extension of the IQS method taking one subdomain and the square root of the static adjoint flux ϕ_0^* as weight function. In our multi-domain case, the normalization condition becomes local on each subdomain :

$$\int_\Omega\frac{1}{V^g}\frac{\partial f}{\partial t}\psi_0^2B_i^{(0)}B_{i'}^{(0)}\overrightarrow{dr}=0\ \ \forall i,i'.\tag{11}$$

Here too, we can find again the IQS condition if the basis function is constant on the single mesh (if the finite elements order is zero). Therefore, the shape time differential term disappears in the equation (8). This condition can be interpreted as an hypothesis of weak variation in time of the condensed shape. That is also why, the other condensed terms, including the shape, are supposed, in a first time, constant during a coarse time step. Eventually, we could iterate on the coarse time step in order to introduce a more accurate time dependence for the shape. Presently, we use a constant weight function : $\psi_0 = 1$. But, other choices will be tested in future developments as the adjoint flux, the adjoint shape or the previous reconstructed flux. This choice could improve the normalization condition and the resulting suppositions.

The obtained small linear system has the same properties than the system which corresponds to the reference method. So, it is solved with the same solver. In the same time, the condensed precursor concentration is computed with the equation (10). In MINOS solver, the precursor equation is solved exactly in time. In amplitude calculations, it is a condensed concentration $\int_\Omega c\chi_d\psi_0B_{i'}^{(0)}\overrightarrow{dr}$, in the condensed equation (10), which is solved exactly in time. It is possible because we suppose that the weight function and the basis functions are constant in time.

3.2. Shape Calculation

When one solves the shape equations (6), the amplitude is known for the whole coarse time step. The shape is computed on the fine space mesh, associated to the global flux, and for the coarse time step. So, to solve (6) is equivalent to find, for each group g, $f^g \in L^2(\Omega)$ and
$\overrightarrow{p_f^g} \in H(div, \Omega, \Gamma_N) = \{ \overrightarrow{q} \in (L^2(\Omega))^3 / \overrightarrow{\nabla}.\overrightarrow{q} \in L^2(\Omega) / \overrightarrow{q}.\overrightarrow{n} = 0 \,\text{on}\, \Gamma_N \}$ such as :

$$\int_\Omega V^{-1} \frac{\partial(af)}{\partial t} \psi \overrightarrow{dr} = -\int_\Omega \overrightarrow{\nabla}.\overrightarrow{p_f} \psi \overrightarrow{dr} - \int_\Omega (\Sigma_t - \chi\nu\Sigma_f - \Sigma_s)\, af\psi \overrightarrow{dr} + \int_\Omega S_e(c,a)\psi \overrightarrow{dr}\,,$$
$$\int_\Omega (aD)^{-1} \overrightarrow{p_f}.\overrightarrow{q}\, \overrightarrow{dr} - \int_\Omega f \overrightarrow{\nabla}.\overrightarrow{q}\, \overrightarrow{dr} + \int_{\Gamma_R} (a[\tau])^{-1} (\overrightarrow{p_f}.\overrightarrow{n})(\overrightarrow{q}.\overrightarrow{n}) ds = 0\,, \tag{12}$$

$\forall \psi \in L^2(\Omega)$ and $\forall \overrightarrow{q} \in H(div, \Omega, \Gamma_N)$. Thus, the shape and the amplitude are both computed with the reference solver but for different space and time discretizations. The specificity of this resolution is to condense the data in time. To integrate a coarse time step, we subdivide it on a sum of the thin steps on which we have computed the amplitude.

It is interesting to see how each function contributes to the other problem. As in the amplitude equations, one find again neutronic data multiplied by an integrated function (here, it is the amplitude) and an additional extern source which is the leakage associated to the amplitude. But moreover, in this problem, we have a boundary source corresponding to the Robin current condition.

3.3. Resulting Algorithm

The fine time steps are chosen in order to be a subdivision of the coarse step. So the sequencing of the resolution can be summarized as follows :

1 - Initialization of the flux, the precursor concentration and the factorization ($f^g = \phi^g$ and $a^g = 1$);
2 - For the coarse time steps :
  a - For each fine time step included in the considered coarse step :
    i - Resolution of the condensed amplitude problem (8);
    ii - Calculation of the condensed precursor concentration with equation (10);
  b - Resolution of the shape problem (6);
  c - Calculation of the precursor concentration on the coarse time steps;
3 - Reconstructing of the global flux with factorization (3) for each time.

As we have already say, we could iterate on the thin time step in order to improve the shape time approximation. For example, a first loop enables an estimation of a linear coarse evolution.

4. FIRST TESTS AND RESULTS

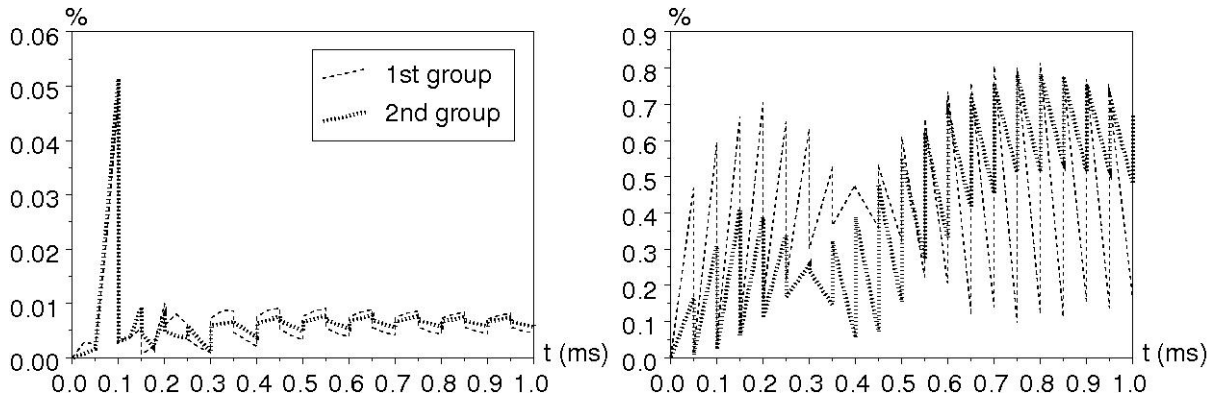
We test our method in two steps. Firstly, we realize a simplified implementation for an one dimension problem. In order to validate the theory, we look at the consistency and a first validation in this case. Secondly, we implement the method in a more global 3D code. These tests are pending but they will be in our oral presentation.

4.1. The Adaptation of the TWIGL Benchmark

The first tests have been performed on a simplified benchmark, derived from the TWIGL benchmark [6] reduced to one dimension. On an axial view ($200cm$), there are three different compositions : reflector on bottom ($20cm$) and top ($20cm$), fuel ($80cm$) and absorber ($80cm$) which moves to the top and is replaced by the fuel. There are two energy groups.We have made two principal tests with these data. The first shows the computing evolutions in a static situation and the second simulates an absorber ejection (the absorber disappears in $1ms$).

4.2. A Numerical Proof of Consistency

For this first case, since the flux is initialized with a critical stationary flux ($k_{eff} = 1$) and the neutronic data do not change, the flux remains constant during the time. This result is well observed on figure 1(a) which represents the error between the initial flux and the flux computed with the LQS method for two subdomains, two fine time steps per coarse step and a constant weight function. Similar results are observed with more subdomains and with more fine time steps per coarse step.



(a) The Static Case (b) The Absorber Ejection Case

Figure 1. Relative Error in Percentage on the Flux Peak Obtained with the LQS Method

4.3. A First Validation of the Approach

The second case is a simulation of a rod ejection for this one dimensional reactor. For $t = 0s$, the axial composition is $80cm$ of fuel and $80cm$ of absorbent. At the end ($t = 0.001s$), the axial composition becomes $160cm$ of fuel and $0cm$ of absorbent. The evolution of the relative error of the flux peak is represented on the figure 1(b). One can observe that this error is small ($< 1\%$).

4.4. The 3D results

We are implementing and testing our method in a more global 3D code. We will be able to present the results during the meeting. For example, we will compare the LQS method to the reference solver in order to see the interest of this approach.

5. CONCLUSIONS AND PERSPECTIVES

We have introduced a new multi-scale approach. The first numerical results illustrate the pertinence of the modeling. These results are incomplete and there are some theoretical elements which have not been yet included as a more judicious weight function. A complete 3D code is under development with more possibilities to improve the efficiency of our Local Quasi-Static method.

Nevertheless, some advantages can be already considered. The code is fast and could have an adaptable precision (with more or less subdomains) at a low CPU time. In fact, in the amplitude resolution, it is the matrix construction which is expansive in computing time. But this time is independent of the number of subdomains. Furthermore, the assembling is local for each subdomain and so it can be easily parallelized. There are also possibilities to extend the method to adaptive scales, for time and space, easier than for the reference solver (because the method is developed for multi-scale considerations). These elements are being investigated and will be presented in a next paper.

REFERENCES

[1] A.M. Baudron and J.J. Lautard, "MINOS : a SPN solver for core calculation", *Nuclear Science and Engineering*, **155**, Number 2, pp. 250-263 (2007).

[2] A.M. Baudron, J.J. Lautard, M. Dahmani and L. Erradi, "Application of the nodal mixed dual technique of spatial reactor kinetics using the improved quasi-static method," *Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications*, Madrid, Spain, September 27-30 (1999).

[3] M. Dahmani, "Résolution des équations de la cinétique des réacteurs nucléaires par la méthode nodale mixte duale utilisant le modèle quasi-statique amelioré et implémentation dans le code CRONOS," *PhD Thesis, Faculté des sciences de Rabat, Maroc* (1999).

[4] R. Dautray and J.L. Lions, *Analyse mathématique et calcul numérique*, Masson, Paris, France (1984).

[5] J. Planchard, *Méthodes mathématiques en neutronique*, Éditions EYROLLES, Collection de la Direction des Études et Recherches d'EDF, Paris, France (1995).

[6] S. Langenbuch, W. Maurer and W. Werner, "Coarse-Mesh Flux-Expansion Method for the Analysis of Space-Time Effects in Large Light Water Reactor Cores," *Nuclear Science and Engineering*, **63**, pp. 437-456 (1977).

[7] K.O. Ott and D.A. Meneley, "Accuracy of the quasistatic treatment of spatial reactor kinetics," *Nuclear Science and Engineering*, **36**, pp. 402-411 (1969).

[8] P.-A. Raviart and J.M. Thomas, "A mixed finite element method for 2nd order elliptic problems," *Lecture Notes in Math., Mathematical aspects of finite element methods (Proc. Conf., Consiglio Naz. delle Ricerche (C.N.R.)*, Rome, 606, 292-315 (1975).

[9] R. Sanchez, C. Magnaud, J.J. Lautard, D. Caruge et alter, "SAPHYR : A Code System from Reactor Design to Reference Calculations," *International Conference on Supercomputing in Nuclear Applications*, Paris, France (2003).