ON THE APPLICATION OF AN ADJOINT RESHUFFLING-INVARIANT NUCLIDE DENSITY FIELD FOR ACCELERATING EQUILIBRIUM CYCLE ITERATIONS

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ABSTRACT

As nuclear fuel economy is basically a multi-cycle issue, a fair way of evaluating reload patterns is to consider their performance in the case of an *equilibrium cycle*. The equilibrium cycle associated with a reload pattern is defined as the limit fuel cycle that eventually emerges after multiple successive periodic refueling, each time implementing the same reload scheme. Since the equilibrium cycle is the solution of a reload operation invariance equation, it can in principle be found with sufficient accuracy only by applying an iterative procedure, simulating the emergence of the limit cycle. For a design purpose such as the optimization of reload patterns, in which many different equilibrium cycle perturbations (resulting from many different limited changes in the reload operator) must be evaluated, this requires large computational efforts. For enabling faster evaluation of these many different equilibrium cycle perturbations it is possible to set up a generalized perturbation theory approach. This approach results in an iterative scheme that yields the *exact* perturbation in the equilibrium cycle solution as well in an accelerated way, thus establishing a speed-up of the equilibrium cycle convergence. Furthermore, the solution of the adjoint equations occurring in the formalism has been *parallellized* and executed on a massively parallel machine. The combination of generalized perturbation theory and parallellism (assuming also that an inherently parallel loading pattern optimization procedure can be applied) will offer the opportunity to establish a significant speed-up for the sampling of the solution space for the equilibrium cycle reload pattern optimization problem.

1. GENERALIZED EQUILIBRIUM CYCLE DEPLETION PERTURBATION THEORY

Since the time dependent neutronics and nuclide density fields implicitly depend on one another, a spatial perturbation in the nuclide density field at BOC (so at $t=t_0^+$) will perturb the entire neutron/nuclide field for the forthcoming cycle. In classical depletion

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perturbation theory (DPT) (Williams 1979), it is conventionally assumed that the perturbed BOC nuclide density distribution is known exactly. Due to the fact that the neutronics field and the nuclide density field are governed by a set of coupled (differential) equations and cannot be varied independently, it is impossible to calculate directly the exact way in which a perturbation in the combined neutron/nuclide field will propagate from BOC to EOC. Any data change that changes one field will also change the other field, because the two fields are constrained to "move" only in a fashion consistent with their coupled field equations. Yang and Downar (Yang, 1989) developed depletion perturbation theoretical methods for the equilibrium cycle, in order to assess the effects of changes in general reactor physics parameters (such as material properties or the enrichment level of fresh fuel assemblies) for a fixed reload pattern. However, for application in for example loading pattern optimization, it is of course necessary to consider changes in a far more abstract, discrete equilibrium cycle parameter, which is *the reload pattern itself*. The reload operator can be represented mathematically by a square binary matrix $\mathbf{X}$, the elements of which are to be defined by

$$\mathrm{X_{IJ}} = \begin{cases} 1 & \text{if the fuel element that has resided in node J} \\ & \text{is located in node I after reloading} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

If $\sum_{\mathrm{I}} \mathrm{X_{IJ}} = 0$ then obviously the fuel element that has resided in node J is to be discharged. If $\sum_{\mathrm{J}} \mathrm{X_{IJ}} = 0$, then apparently none of the older fuel elements which were already present in the core will be place in node I during reloading. In that case, node I is to receive a fresh fuel element. If the fuel elements are characterized by their nuclide density vectors, the invariance of the equilibrium cycle with respect to the reload operation can be mathematically defined as:

$$\underline{\underline{\mathrm{N}}}(\mathrm{t}_0^+) \;=\; \mathbf{X}\,\underline{\underline{\mathrm{N}}}(\mathrm{t}_{\mathrm{T}}^-) \;+\; (\mathbf{1}-\mathbf{X})\,\underline{\underline{\mathrm{N}}}_{\mathrm{F}} \tag{2}$$

$\underline{\underline{\mathrm{N}}}_{\mathrm{F}}$ is a convenient notation for $(\underline{\mathrm{N}}_{\mathrm{F}}, \underline{\mathrm{N}}_{\mathrm{F}}, ..., \underline{\mathrm{N}}_{\mathrm{F}})^{\mathrm{T}}$ with $\underline{\mathrm{N}}_{\mathrm{F}}$ the vector denoting the densities of the different nuclides in the fresh fuel. The symbol **1** indicates the unity operator. The equilibrium cycle can be determined iteratively using this invariance condition. All the system equations, governing the equilibrium cycle burnup physics for the core, can be treated as constraints on the response, and appended to the response function using appropriate Lagrange multipliers. Since the reload operation takes place in the nuclide density space, the reload equation will have the same Lagrange multiplier as the nuclide transmutation equation. First of all, we note that the transmutation equation dictating the time evolution of the nuclide density field can be written as

$$\frac{\partial}{\partial \mathrm{t}}\underline{\underline{\mathrm{N}}}(\mathrm{t}) = \left(\hat{\sigma}\underline{\phi}(\mathrm{t}) + \hat{\mathrm{D}}\right)\underline{\underline{\mathrm{N}}}(\mathrm{t}) \tag{3}$$

with $\hat{\sigma}$ denoting the absorption cross sections matrix and $\hat{D}$ the decay operator. We emphasize here that the operators active in the *nuclide type space* are marked with a hat, and that an implicit product in the nuclide type space occurs when the operators $\hat{\sigma}$ and $\hat{D}$

appear in combination with the nuclide density field $\underline{\underline{\mathrm{N}}}$ (t). The flux $\underline{\phi}$(t) can be written as a product of the time dependent shape function $\psi(\mathbf{r},\mathrm{t})$ (which is normalized such that $\int \psi(\mathbf{r},\mathrm{t})\mathrm{dV} = 1$ for all t) and a time dependent power normalisation factor $\Phi(\mathbf{r},\mathrm{t})$. This allows for a convenient implementation of the condition that the reactor power is restricted to remain at a constant level. In inner product notation, this condition can be written as:

$$\mathrm{w_f}\Phi_\mathrm{i}\langle\underline{\underline{\Sigma}}_{\mathrm{F,i}}|\underline{\psi}_\mathrm{i}\rangle = \mathrm{P_{total}} \text{ for all } \mathrm{i} = 0,...\mathrm{T}-1 \tag{4}$$

where it becomes clear that a quasi-static burnup approach has been adopted, featuring T equidistant time intervals. For each time interval [$\mathrm{t_i}$,$\mathrm{t_{i+1}}$] the flux shape λ-eigenvalue equation is satisfied:

$$(\mathbf{L}_\mathrm{i} - \lambda_\mathrm{i}\mathbf{F}_\mathrm{i})\,\underline{\psi}_\mathrm{i} = \underline{0} \tag{5}$$

where the eigenvalue λ is the reciprocal of the effective multiplication factor of the uncontrolled (=without external reactivity control) core $\mathrm{k_{eff}}$ and $\mathbf{L}$ and $\mathbf{F}$ are the loss and production operator, respectively. The response quantity we are interested in is the full collection of all nuclide densities at the end of the operation cycle, so defined at t=$\mathrm{t_T^-}$. In order to stress that the response is defined at t=$\mathrm{t_T^-}$, we denote the response quantity as $\underline{\underline{\mathrm{N}}}(\mathrm{t_T^-})$. Applying the Lagrange multipliers $\hat{\Gamma}_\mathrm{i}^*$, $\mathbf{P}_\mathrm{i}^*$ and $\mathbf{N}^*$(t), the general response functional $\mathcal{R}\left[\mathbf{X}, \underline{\underline{\mathrm{N}}}(\mathrm{t}), \underline{\underline{\mathrm{N}}}_\mathrm{F}, \underline{\psi}_\mathrm{i}, \Phi_\mathrm{i}, \lambda_\mathrm{i}\right]$ can be written as:

$$\begin{aligned}\mathcal{R} = \underline{\underline{\mathrm{N}}}(\mathrm{t_T^-}) &+ \sum_{\mathrm{i}=0}^{\mathrm{T}-1}\int_{\mathrm{t_i}}^{\mathrm{t_{i+1}}}\left\langle \mathbf{N}^*(\mathrm{t})\middle|\hat{\sigma}\Phi_\mathrm{i}\underline{\psi}_\mathrm{i} + \hat{\mathrm{D}} - \frac{\partial}{\partial \mathrm{t}}\middle|\underline{\underline{\mathrm{N}}}(\mathrm{t})\right\rangle \mathrm{dt} \\ &- \sum_{\mathrm{i}=0}^{\mathrm{T}-1}\langle\hat{\Gamma}_\mathrm{i}^*|(\mathbf{L}_\mathrm{i} - \lambda_\mathrm{i}\mathbf{F}_\mathrm{i})\underline{\psi}_\mathrm{i}\rangle - \sum_{\mathrm{i}=0}^{\mathrm{T}-1}\mathbf{P}_\mathrm{i}^*\left(\mathrm{w_f}\Phi_\mathrm{i}\langle\underline{\underline{\Sigma}}_{\mathrm{F,i}}|\underline{\psi}_\mathrm{i}\rangle - \mathrm{P_{total}}\right) \\ &+ \int_{\mathrm{t_T^-}}^{\mathrm{t_T^+}}\left\langle \mathbf{N}^*(\mathrm{t})\middle| - \frac{\partial}{\partial \mathrm{t}}\underline{\underline{\mathrm{N}}}(\mathrm{t}) + (\mathbf{X}-\mathbf{1})(\underline{\underline{\mathrm{N}}}(\mathrm{t}) - \underline{\underline{\mathrm{N}}}_\mathrm{F})\delta(\mathrm{t}-\mathrm{t_T})\right\rangle \mathrm{dt}\end{aligned} \tag{6}$$

in which the integrand in the last term is the differential equation describing the reload operation at EOC. The symbol **1** represents the unity operator. Forward integration of this equation from $\mathrm{t_T^-}$ to $\mathrm{t_T^+}$ yields the reload equation (2). If $\underline{\underline{\mathrm{N}}}(\mathrm{t})$, $\underline{\psi}_\mathrm{i}$, λ_i and Φ_i are exact equilibrium cycle solutions to the quasi-static burnup equations, then $\mathcal{R} = \underline{\underline{\mathrm{N}}}(\mathrm{t_T^-})$. Now, if the reload operator $\mathbf{X}$ and the fresh fuel composition $\underline{\mathrm{N}}_\mathrm{F}$ (and hence the entire equilibrium cycle solution) are perturbed, this will influence $\mathcal{R}$:

$$\mathcal{R} \rightarrow \mathcal{R}'(\mathbf{X}', \underline{\underline{\mathrm{N}}}'(\mathrm{t}), \underline{\underline{\mathrm{N}}}'_\mathrm{F}, \underline{\psi}'_\mathrm{i}, \Phi'_\mathrm{i}, \lambda'_\mathrm{i}), \tag{7}$$

where the prime variables refer to their perturbed values. Again, if $\underline{\underline{\mathrm{N}}}'(\mathrm{t})$, $\underline{\psi}'_\mathrm{i}$, Φ'_i and λ'_i exactly satisfy the perturbed equilibrium cycle system equations dictated by $\mathbf{X}'$ and $\underline{\mathrm{N}}'_\mathrm{F}$,

then $\mathcal{R}' = \underline{\underline{\mathrm{N}}}'(\mathrm{t}_\mathrm{T}^-)$, so the perturbed functional value will be equal to the exact perturbed EOC equilibrium cycle nuclide density distribution. Expanding $\delta\mathcal{R}$ about the unperturbed state and neglecting the second-order terms in the continuous variables, we obtain the first-order prediction for $\delta\mathcal{R}$, denoted as $\delta^{(1)}\mathcal{R}$:

$$\delta^{(1)}\mathcal{R} = \delta\underline{\underline{\mathrm{N}}}(\mathrm{t}_\mathrm{T}^-) + \sum_{\mathrm{i}=0}^{\mathrm{T}-1}\left\{\int_{\mathrm{t_i}}^{\mathrm{t_{i+1}}}\left\langle\frac{\partial\mathcal{R}_1}{\partial\underline{\underline{\mathrm{N}}}(\mathrm{t})}\middle|\delta\underline{\underline{\mathrm{N}}}(\mathrm{t})\right\rangle\mathrm{dt} + \frac{\partial\mathcal{R}_1}{\partial\lambda_\mathrm{i}}\delta\lambda_\mathrm{i} + \frac{\partial\mathcal{R}_1}{\partial\Phi_\mathrm{i}}\delta\Phi_\mathrm{i} + \left\langle\frac{\partial\mathcal{R}_1}{\partial\underline{\psi}_\mathrm{i}}|\delta\underline{\psi}_\mathrm{i}\right\rangle\right\}$$

$$+\int_{\mathrm{t}_\mathrm{T}^-}^{\mathrm{t}_\mathrm{T}^+}\left\langle\mathbf{N}^*(\mathrm{t})\middle|\frac{\partial}{\partial\mathrm{t}}\delta\underline{\underline{\mathrm{N}}}(\mathrm{t}) + \left[\mathbf{X}'\delta\underline{\underline{\mathrm{N}}}(\mathrm{t}) + \delta\mathbf{X}\underline{\underline{\mathrm{N}}}'(\mathrm{t}) - \delta\mathbf{X}\underline{\underline{\mathrm{N}}}_\mathrm{F} + (\mathbf{1}-\mathbf{X}')\delta\underline{\underline{\mathrm{N}}}_\mathrm{F}\right]\delta(\mathrm{t}-\mathrm{t}_\mathrm{T})\right\rangle\mathrm{dt} \tag{8}$$

Many of the contributions to $\delta^{(1)}\mathcal{R}$ can be forced to vanish by defining the Euler-Lagrange stationarity equations for the adjoint fields $\hat{\Gamma}_\mathrm{i}^*$, $\mathbf{P}_\mathrm{i}^*$ and $\mathbf{N}^*(\mathrm{t})$ (Williams, 1979, Yang, 1989, Van Geemert, 2001):

$$\frac{\partial\mathcal{R}}{\partial\Phi_\mathrm{i}} = 0 \implies \mathbf{P}_\mathrm{i}^* = \frac{1}{\mathrm{w_f}\left\langle\underline{\Sigma}_{\mathrm{F,i}}|\underline{\psi}_\mathrm{i}\right\rangle}\int_{\mathrm{t_i}}^{\mathrm{t_{i+1}}}\left\langle\mathbf{N}^*(\mathrm{t})\middle|\hat{\sigma}\underline{\psi}_\mathrm{i}|\underline{\underline{\mathrm{N}}}(\mathrm{t})\right\rangle\mathrm{dt} \tag{9}$$

$$\frac{\partial\mathcal{R}}{\partial\underline{\psi}_\mathrm{i}} = 0 \implies (\mathbf{L}_\mathrm{i}^* - \lambda_\mathrm{i}\mathbf{F}_\mathrm{i}^*)\,\hat{\Gamma}_\mathrm{i}^* = \mathbf{Q}_\mathrm{i}^* \equiv \int_{\mathrm{t_i}}^{\mathrm{t_{i+1}}}\left\langle\mathbf{N}^*(\mathrm{t})\middle|\hat{\sigma}\Phi_\mathrm{i}\middle|\underline{\underline{\mathrm{N}}}(\mathrm{t})\right\rangle\mathrm{dt} - \mathrm{w_f}\mathbf{P}_\mathrm{i}^*\Phi_\mathrm{i}\underline{\Sigma}_{\mathrm{F,i}} \tag{10}$$

$$\frac{\partial\mathcal{R}}{\partial\lambda_\mathrm{i}} = 0 \implies \left\langle\hat{\Gamma}_\mathrm{i}^*\middle|\mathbf{F}_\mathrm{i}\underline{\psi}_\mathrm{i}\right\rangle = 0 \tag{11}$$

The stationarity condition corresponding to a variation in $\underline{\underline{\mathrm{N}}}$(t) is more complex than for the other variables. This is basically because $\underline{\underline{\mathrm{N}}}$(t) is the only 'forward' quantity that is allowed to vary continuously in time. Due to this, a significant part of its contribution in the variation functional is embedded in an integral, whereas the other part merely consists of terms defined at discrete equidistant moments $\mathrm{t_i}$ containing the 'snapshots' $\underline{\underline{\mathrm{N}}}(\mathrm{t_i})$ of the nuclide density fields. These Euler conditions, of which the derivation is described rigorously in (Williams 1979, Yang, 1989, Van Geemert, 2001), are the adjoint transmutation equation

$$\frac{\partial}{\partial\mathrm{t}}\mathbf{N}^*(\mathrm{t}) = -\left(\hat{\sigma}^*\Phi_\mathrm{i}\underline{\psi}_\mathrm{i} + \hat{\mathrm{D}}^*\right)\mathbf{N}^*(\mathrm{t}),\ \ \mathrm{t_i} < \mathrm{t} < \mathrm{t_{i+1}} \tag{12}$$

and the in-cycle time boundary discontinuity conditions :

$$\mathbf{N}^*(\mathrm{t_i^-}) = \mathbf{N}^*(\mathrm{t_i^+}) - \mathbf{z_i}\ \ , \mathrm{i} = 0, 1, ..., \mathrm{T}-2, \tag{13}$$

with the discontinuity terms $\mathbf{z}_\mathrm{i}$ defined as:

$$\mathbf{z_i} = \left\langle\hat{\Gamma}_\mathrm{i}^*\middle|\frac{\partial\mathbf{L_i}}{\partial\underline{\underline{\mathrm{N}}}_\mathrm{i}} - \lambda_\mathrm{i}\frac{\partial\mathbf{F_i}}{\partial\underline{\underline{\mathrm{N}}}_\mathrm{i}}\middle|\underline{\psi}_\mathrm{i}\right\rangle + \mathbf{P}_\mathrm{i}^*\mathrm{w_f}\Phi_\mathrm{i}\left\langle\frac{\partial\underline{\Sigma}_{\mathrm{F,i}}}{\partial\underline{\underline{\mathrm{N}}}_\mathrm{i}}\middle|\underline{\psi}_\mathrm{i}\right\rangle, \tag{14}$$

When these conditions are satisfied, the summation eventually reduces to

$$\delta^{(1)}\mathcal{R}_1\left[\delta\underline{\underline{\mathrm{N}}}(\mathrm{t})\right] = \langle \mathbf{N}^*(\mathrm{t}_0^+) - \mathbf{z}_0 | \delta\underline{\underline{\mathrm{N}}}(\mathrm{t}_0^+)\rangle - \langle \mathbf{N}^*(\mathrm{t}_\mathrm{T}^-) | \delta\underline{\underline{\mathrm{N}}}(\mathrm{t}_\mathrm{T}^-)\rangle \tag{15}$$

The condition that the integral part of $\delta\mathcal{R}_2\left[\delta\underline{\underline{\mathrm{N}}}(\mathrm{t})\right]$ disappears results in the following adjoint reload operation differential equation to be satisfied :

$$-\frac{\partial}{\partial \mathrm{t}}\mathbf{N}^*(\mathrm{t}) = \left(\mathbf{X}^*(\mathbf{N}^*(\mathrm{t}) - \mathbf{z}_0) - \mathbf{N}^*(\mathrm{t}) \; + \; \mathbf{1}\right)\delta(\mathrm{t} - \mathrm{t}_\mathrm{T}) \tag{16}$$

Integration of this differential equation from t_T^- to t_T^+ yields the *adjoint cyclic boundary condition* (Van Geemert, 2001) to be satisfied by the adjoint time-dependent nuclide density distribution $\mathbf{N}^*(\mathrm{t})$:

$$\mathbf{N}^*(\mathrm{t}_\mathrm{T}^-) = \mathbf{X}^*(\mathbf{N}^*(\mathrm{t}_0^+) - \mathbf{z}_0) \; + \; \mathbf{1} \tag{17}$$

If this condition is satisfied, $\delta^{(1)}\mathcal{R}$ can be written very compactly as

$$\delta^{(1)}\mathcal{R} = \langle \mathbf{N}^*(\mathrm{t}_0^+) - \mathbf{z}_0 | \delta\mathbf{X}(\underline{\underline{\mathrm{N}}}(\mathrm{t}_\mathrm{T}^-) - \underline{\underline{\mathrm{N}}}'_\mathrm{F}) + (\mathbf{1} - \mathbf{X})\delta\underline{\underline{\mathrm{N}}}_\mathrm{F} + \delta\mathbf{X}\delta\underline{\underline{\mathrm{N}}}(\mathrm{t}_\mathrm{T}^-)\rangle \tag{18}$$

We stress that the principal part of this first-order prediction $\delta^{(1)}\mathcal{R}$ of the perturbed equilibrium cycle EOC field,

$$\langle \mathbf{N}^*(\mathrm{t}_0^+) - \mathbf{z}_0 | \delta\hat{\mathbf{X}}(\underline{\underline{\mathrm{N}}}(\mathrm{t}_\mathrm{T}^-) - \underline{\underline{\mathrm{N}}}'_\mathrm{F}) + (\mathbf{1} - \mathbf{X})\delta\underline{\underline{\mathrm{N}}}_\mathrm{F}\rangle \tag{19}$$

can be obtained directly, *without* any new iterative calculations. Further, it is interesting to point out the physical interpretation of Eq.(17). This physical interpretation is set in a reversed time picture in which importances are propagated from one fuel element position preceding the other in correspondence with an adjoint reload operation. This interpretation is illustrated in Fig.1. Whereas the normal reload scheme indicates in a forward way how disturbances in fresh fuel elements travel through the core via the periodic shuffling process, the adjoint reload scheme indicates (in a backward way) the history of an observed disturbance in a *discharged* fuel element, thus eventually pinpointing from where and when the disturbance originates.

3. GPT-BASED ACCELERATION OF EQUILIBRIUM CYCLE CONVERGENCE

The general numerical goal defined for this study is to develop and implement an *accelerated* way to perform the equilibrium cycle iteration for a modestly perturbed reload operator. In the normal picture this iteration is done by plain simulation of how a limit cycle is reached in real life, i.e. one simply performs the neutronics and depletion calculations during each m^{th} iterated operation cycle, followed by a reloading, each time with the

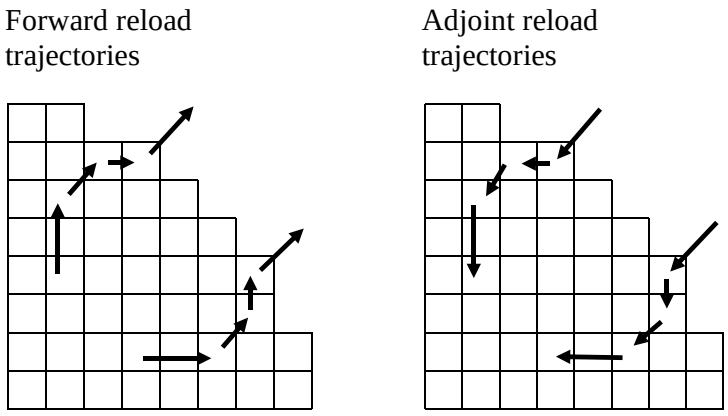

Figure 1 Forward and adjoint reload operations

same reload pattern of which one wants to obtain the associated equilibrium cycle. This process ends when the limit cycle has been obtained with sufficient accuracy. In the numerical picture proposed here, we assume that one forward equilibrium cycle solution has been obtained for a specific reference reload pattern. The reference reload operator and its associated equilibrium cycle solution are assumed to have been adopted as the case for which the adjoint Euler stationarity equations (9), (10) and (11) have been solved. Now, all the new reload operators of which the associated equilibrium cycle solutions need to be evaluated are treated as perturbations on the reference reload operator. If the adjoint cyclic boundary condition (17) is satisfied, the accelerative scheme to be implemented (Van Geemert 2001) can be formulated as

$$\delta^{(\mathrm{m})}_{\mathrm{corr}}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}}) = \delta^{(\mathrm{m})}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}}) + \langle \mathbf{N}^{*}(\mathrm{t}^{+}_{0})|\mathbf{X}'(\delta^{(\mathrm{m})}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}}) - \delta^{(\mathrm{m}-1)}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}}))\rangle \tag{20}$$

The application of this accelerative scheme will, when applied to each newly obtained $\delta^{(\mathrm{m})}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}})$ (with $\delta^{(\mathrm{m})}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}})$ calculated via a perturbed depletion calculation involving the perturbed power distribution), and when applied *before* each standard reload operation yielding the $\delta^{(\mathrm{m}+1)}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{+}_{0})$, result in an *accelerated* convergence towards the exact perturbation in the equilibrium cycle EOC nuclide density distribution, $\delta\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}})$. The more favourable convergence properties arise from the inherently more favourable mathematical structure, especially in the case of modest perturbations. The dependence of the speed-up factor η on $\mathbf{X}$, $\delta\mathbf{X}$ and $\mathbf{N}^{*}(\mathrm{t}^{+}_{0})$ can be formulated as

$$\frac{1}{\eta} = \frac{\parallel \delta^{(2)(\mathrm{m}+1)}_{\mathrm{corr}}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{-}_{\mathrm{T}}) \parallel}{\parallel \delta^{(2)(\mathrm{m})}\underline{\underline{\mathrm{N}}}(\mathrm{t}^{+}_{0}) \parallel} = \parallel (\mathbf{X}+\delta\mathbf{X})^{*}\mathbf{N}^{*}(\mathrm{t}^{+}_{0}) \parallel \tag{21}$$

From the numerical results obtained in our study, of which a few examples are given in section 5, it can be concluded that, for most (magnitudes of) choices for $\delta\mathbf{X}$, $\frac{1}{\eta}$ remains significantly below unity (corresponding to a speed-up) and that the maximum speed-up (which is inversely proportional to $\| (\mathbf{X}+\delta\mathbf{X})^*\mathbf{N}^*(t_0^+) \|$) occurs for $\delta\mathbf{X}=\mathbf{0}$.

4. COMBINATION WITH THE SINGLE TIME-STEP GPT-BASED ACCELERATION OF THE SOLUTION OF THE PERTURBED EIGENVALUE EQUATIONS

In addition to the use of scheme (21) for accelerating the equilibrium cycle convergence, we have set up single time step GPT for achieving significant acceleration of the solution of the λ-eigenvalue equation for the flux shape $\underline{\psi}_i$ for each time-step i. The application of this methodology involves the solution of simpler adjoint fields (like Eq.(10) but with different source terms) that require less computational effort and data management to be acquired and stored, because of the absence of a iterative time loop in the solution process. Since this paper focusses on equilibrium cycle depletion perturbation theory, we will not discuss single time step GPT in detail here. It has already been applied successfully in non-equilibrium core management optimization and is discussed extensively in (Maldonado 1995, Moore 1998, van Geemert 2001).

5. PARALLEL NUMERICAL SOLUTION OF THE ADJOINT FIELDS $\mathbf{N}^*$(t)

The only difficulty in solving the $\hat{\Gamma}_i^*$ from the inhomogeneous equation (10) arises from the property of the operator $(\mathbf{L}_i^* - \lambda\mathbf{F}_i^*)$ that it is *singular* in the sense that a fundamental solution (the fundamental adjoint flux $\underline{\psi}_i^*$) exists for the homogeneous equation

$$(\mathbf{L}_i^* - \lambda\mathbf{F}_i^*)\,\underline{\psi}_i^* \;=\; \underline{0} \tag{22}$$

due to which this fundamental solution $\underline{\psi}_i^*$ must be filtered out (Maldonado 1995, Moore 1998, van Geemert 2001) after each iterative step for determining the $\hat{\Gamma}_i^*$. As far as the acquisition of the $\mathbf{N}^*$(t) is concerned, the calculational flow is very similar to that for the forward equilibrium cycle iteration, except that the adjoint burnup calculations and the reload operation itself have to proceed *backward* in time. As is apparent from Eq.(10), the flux adjoint source $\mathbf{Q}_i^*$ at t_i depends on an integral of $\mathbf{N}^*$(t) over the *future* time interval $[t_i,t_{i+1}]$. Further, the final value of $\mathbf{N}^*$(t) at the end of each time interval is fixed by the discontinuity condition (13). Its magnitude depends not only on the future behaviour of $\mathbf{N}^*$(t) but also on the Γ_i^* and $\mathbf{P}_i^*$ defined at the *final* time of the interval. For the backward solution of the adjoint limit cycle iterations for determining $\mathbf{N}^*$(t), the flow chart depicted in Fig.2 can be implemented.

We note here that the $\mathbf{N}^*$(t) can be thought of as the collection of fully decoupled individual adjoint nuclide density fields $\underline{\underline{N}}_{Jq}^*$ (t) corresponding to the response quantities $N_{Jq}(t_T^-)$ (that is, the equilibrium cycle EOC nuclide density of nuclide type q in node J):

$$\mathbf{N}^*(t) = \left\{ \underline{\underline{N}}_{Jq}^*(t);\, J = 1,...,M, q = 1,...,l \right\} \tag{23}$$

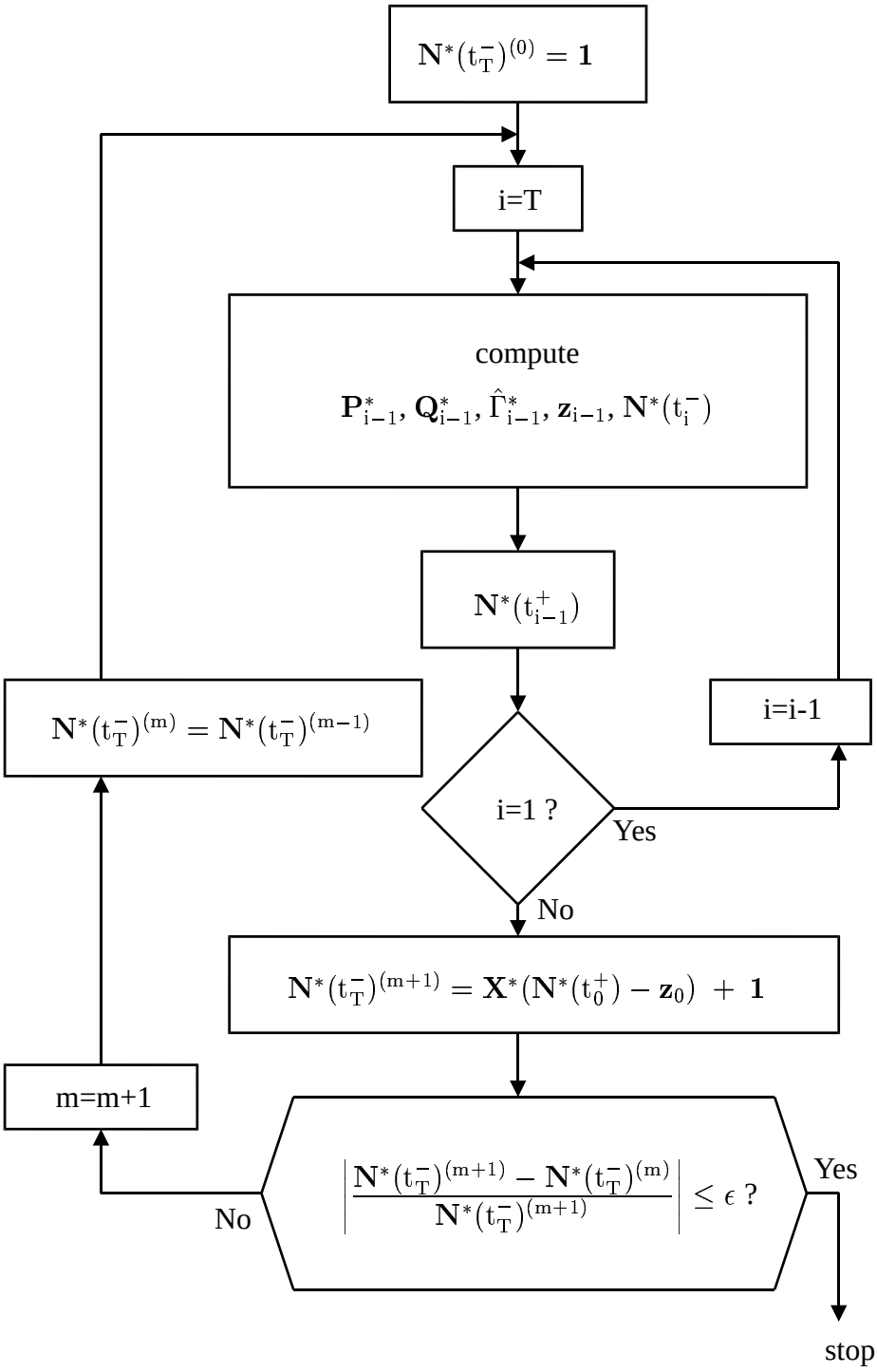

Figure 2 Backward flow chart for iterative calculation of $\mathbf{N}^*(t_0^+)$ such that the adjoint cyclic boundary condition (15) is satisfied

with M the total number of response nodes (fuel assemblies) in the octant and l the number of different nuclide types considered. The *parallellisation* of the calculation of $\mathbf{N}^*(t)$ simply consists of distributing the calculation of the different adjoint field collections $\underline{\underline{N}}^*_{Jq}(t)$ over different parallel processors.

6. RESULTS

The formalism described here has been programmed in MPI-Fortran and implemented on the massively parallel computer available at Delft University of Technology. Some examples have been isolated of reload operator perturbations of different magnitudes, involving binary, ternary, 6-fold and 10-fold interchanges of elements in the reference reload operator for an octant of an octant-symmetric PWR core containing effectively 48 fuel elements per octant. For these examples, we have accelerated the perturbed equilibrium cycle calculations by applying the EOC correction (20) prior to each implementation of the reload operation that can be written in terms of nuclide density perturbations as

$$\delta^{(m+1)}\underline{\underline{N}}(t_0^+) = \delta\mathbf{X}(\underline{\underline{N}}(t_T^-) - \underline{\underline{N}}_F) + \mathbf{X}'(\delta\underline{\underline{N}}^{(m)}_{corr}(t_T^-) - \delta\underline{\underline{N}}_F) + \delta\underline{\underline{N}}_F \qquad (24)$$

In table I, the numbers of iterative steps required for reaching the same prespecified convergence level are listed for the different considered cases, consisting of reload operator perturbations of different magnitudes, involving binary, ternary, 6-fold and 10-fold interchanges of elements in the reference octant-symmetric reload operator $\mathbf{X}$.

Table I Average numbers of required iterative steps for achieving equilibrium cycle convergence ($\epsilon_{EC} \leq 10^{-5}$), with and without application of the EOC-correction (18)

magnitude of permutation	accelerated	non-accelerated
zero	3	12
binary	4	12
ternary	4	12
6-fold	5	12
10-fold	6	12

In the *sequential* implementation for the octant PWR core (featuring 52 response nodes in the octant), the acquisition of $\mathbf{N}^*(t_0^+)$ took about 30 times as much time as one forward equilibrium cycle iteration, per response nuclide type. So obviously (and as expected), the computation of the adjoint fields certainly requires a non-trivial amount of computational effort ! However, for a design purpose such as reload pattern optimization, this investment pays off extremely well in the case where there are very large numbers of pattern changes to be evaluated. If these evaluations can be accelerated considerably using the obtained adjoint fields, the gain in computational efficiency will be significant indeed. Obviously, the computation of $\mathbf{N}^*(t_0^+)$ is embarrassingly parallel, due to which, when n parallel processors can be applied, a decrease of roughly a factor of n in calculation waiting time will

result. This, combined with the application of an parallellised loading pattern optimization algorithm, offers the opportunity to perform exhaustive, fast and accurate sampling of the solution space for the equilibrium cycle optimization problem.

7. CONCLUSIONS

We conclude that the GPT-based equilibrium cycle convergence acceleration method described in this paper is well applicable for acceleration of a heuristic equilibrium cycle optimization procedure that is based on assessing the effects of many different modest permutations in the loading scheme. By this application, a considerable reduction of the number of necessary equilibrium cycle iterations can be realized. The price to be paid, the necessity of solving an extensive set of adjoint equations a few times during the search procedure, will generally pay off easily if the equilibrium cycle convergences occurring in the evaluations of several thousands of candidate schemes can be significantly accelerated using the adjoint fields $\mathbf{N}^*$ (t_0^+). From the obtained speed-up results that could be realized, it can be concluded that the combination of generalized perturbation theory and parallellism (assuming also that an inherently parallel loading pattern optimization procedure can be applied) will offer the opportunity to establish a significant speed-up for the sampling of the solution space for the equilibrium cycle optimization problem.

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