# Application of Quasi-Static Method to Whole Core Transient Calculation in nTRACER

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## 1. Introduction

The direct whole core calculation code nTRACER performs 3D sub-pin level transient calculation for high fidelity multi-physics reactor simulation [1]. In order to alleviate the heavy computational burden, the quasi-static method is implemented to nTRACER. This method has been used to several reactor dynamics applications for efficient transient calculation [2, 3]. By factorizing neutron flux into only time-dependent fast varying amplitude and slow varying shape, larger time-step size is used for expensive shape calculation while maintaining solution accuracy.

Most implementations of the quasi-static method in reactor dynamics come in two major variations, namely, improved quasi-static (IQS) method and predictor-corrector quasi-static (PCQS) method. IQS solves the nonlinear system of the shape and amplitude equations while PCQS linearly corrects the flux level with amplitude [2]. By avoiding the computational cost from nonlinear iteration, PCQS usually shows better computational efficiency and even shows better accuracy in several cases. Both IQS and PCQS are examined with nTRACER. In addition the exponential transformation (ET) method [4] that assumes an exponential variation of the regional flux is investigated noting that ET resembles IQS in that it applies the temporal discretization to the factorized component. There were several applications of quasi-static methods to the diffusion solvers [2] and PCQS application to pin-resolved transport solution [3]. This work examined the applicability of IQS to the sub-pin level transport calculation of nTRACER noting that it already uses nonlinear iteration for convergence of whole core transport solution. The characteristics and effectiveness of the three methods (IQS, PCQS and ET) are also compared and analyzed in the work here.

## 2. Quasi-Static Approaches

The time-dependent neutron balance equation is written in operator form as

$$\begin{cases} \dfrac{1}{v}\dfrac{\partial \Phi}{\partial t} = -\mathbf{M}\Phi + (\mathbf{F}-\mathbf{F}_d)\Phi + S_d \\ \dfrac{\partial \mathbf{C}_k}{\partial t} = \mathbf{F}_{dk}\Phi - \lambda_k \mathbf{C}_k, \ k=1,...,K. \end{cases} \quad (1)$$

Where $\Phi$ is the neutron scalar flux, $\mathbf{C}_k$ is the delayed neutron precursors density for precursor group

$k$. The symbol $\mathbf{M}$ is migration and loss operator, $\mathbf{F}$ and $\mathbf{F}_d$ represent static fission production and quasi-stationary delayed neutron production respectively. $S_d$ denotes actual delayed neutron source.

The quasi-static method is based on a factorization of the neutron flux into two components, 'amplitude' and 'shape':

$$\phi(\mathbf{r},E,t) = p(t)\tilde{\phi}(\mathbf{r},E,t). \quad (2)$$

The amplitude $p(t)$ represents overall amplitude changes of neutron flux and it is only dependent on time. The shape function $\tilde{\phi}(\mathbf{r},E,t)$ still depends on all variables but it has comparatively small time variation than the neutron flux. For unique factorization, the constraint condition is required. The normalization condition weighted with initial adjoint flux $\Phi_0^*$ can be used as the constraint condition:

$$(\Phi_0^*, \frac{1}{v}\tilde{\Phi}) = K_0, \quad (3)$$

where the initial value $K_0 = (\Phi_0^*, \frac{1}{v}\Phi_0)$ is constant.

Applying factorization in Eq. (2) into the Eq. (1) yields the time-dependent shape equation:

$$\frac{1}{v}\frac{\partial \tilde{\Phi}}{\partial t} = -\mathbf{M}\tilde{\Phi} + (\mathbf{F}-\mathbf{F}_d)\tilde{\Phi} + \frac{1}{p}\left[ S_d - \frac{1}{v}\tilde{\Phi}\frac{dp}{dt} \right]. \quad (4)$$

With known $p(t)$ and its time derivative term, shape component can be computed by integrating Eq. (4). On the other hand, integrating Eq. (1) with weighting function $\Phi_0^*$ yields exact point kinetics equation (PKE):

$$\begin{cases} \dfrac{dp}{dt} = \dfrac{\rho(t)-\beta(t)}{\Lambda(t)}p(t) + \dfrac{1}{\Lambda_0}\sum_k \lambda_k \zeta_k(t) \\ \dfrac{d\zeta_k}{dt} = -\lambda_k \zeta_k(t) + \dfrac{F(t)}{F_0}\beta_k(t)p(t), \ k=1,...K, \end{cases} \quad (5)$$

with PKE parameter set defined as

$$\Lambda(t) = (\Phi_0^*, \frac{1}{v}\tilde{\Phi})/(\Phi_0^*, \mathbf{F}\tilde{\Phi}), \quad (6)$$

$$\rho(t) = (\Phi_0^*, [\mathbf{F} - \mathbf{M}]\tilde{\Phi}) / (\Phi_0^*, \mathbf{F}\tilde{\Phi}), \qquad (7)$$

$$\beta(t) = (\Phi_0^*, \mathbf{F}_d\tilde{\Phi}) / (\Phi_0^*, \mathbf{F}\tilde{\Phi}), \qquad (8)$$

$$\zeta_k(t) = (\Phi_0^*, \chi_{dk}C_k) / (\Phi_0^*, \mathbf{F}\tilde{\Phi}). \qquad (9)$$

The amplitude can be computed by integrating Eq. (5) with knowledge of PKE parameters in Eqs. (6)-(9). Since integration of PKE equation doesn't impose heavy computational cost, temporal discretization with micro time-step $\delta t$, which is much smaller than macro time-step $\Delta t$ used for discretization of shape derivative, is possible. However PKE parameters are dependent on the shape. Therefore evaluation of PKE parameters should be accompanied by accurate computation of shape.

*2.1 Improved Quasi-Static Method*

In advance, it was shown that the shape equation Eq. (4) and PKE equation (5) are nonlinearly coupled. IQS directly solve this nonlinearly coupled system with iterative method. Following is typical algorithm of IQS involving Picard iteration:

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**Algorithm 1  IQS algorithm**

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1:   **do** $i = 1, 2 \dots$ until convergence,
2:      Evaluate $\tilde{\Phi}_i$ from Eq. (4) with $\Delta t$
3:      Generate PKE parameters in Eqs. (6)-(9)
4:      Update $p_i$ by solving Eq. (5) with $\delta t$
5:      Get corrected $\Phi_i$ with updated $p_i$
6:   **end do**
7:      $t = t + \Delta t$

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Above algorithm doesn't guarantee the constraint condition in Eq. (3) until it is fully converged. Some implementations of IQS guarantee constraint condition by rescaling the shape function after step 3 in above algorithm with the factor $K_0 / (\Phi_0^*, \frac{1}{v}\tilde{\Phi}_i)$ [2].

*2.2 Predictor Corrector Quasi-Static Method*

Unlike IQS, the concept of flux factorization is maintained but Eq. (4) is not solved in PCQS. The shape is computed from the neutron flux with constraint condition in Eq. (3). Therefore the constraint condition is always preserved in PCQS. The algorithm of PCQS could be presented as

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**Algorithm 2  PCQS algorithm**

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1:   Predict $\Phi_p$ by solving Eq. (1) with $\Delta t$
2:   Factorize $\Phi_p$ into $p_p$ and $\tilde{\Phi}$ based on Eq. (3)

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$$p_p = (\Phi_0^*, \frac{1}{v}\Phi_p) / K_0, \quad \tilde{\Phi} = \frac{1}{p_p}\Phi_p$$

3:   Generate PKE parameters in Eqs. (6)-(9)
4:   Update corrected $p_c$ by solving Eq. (5) with $\delta t$
5:   Get corrected $\Phi_c = p_c\tilde{\Phi}$
6:      $t = t + \Delta t$

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The low subscript 'p' and 'c' in above algorithm represents predictor and corrector respectively. This algorithm assumes that the shape function calculated with macro time-step $\Delta t$ is accurate enough. PCQS doesn't require nonlinear iteration since the solution of the time-dependent neutron balance equation (1) can't be improved with corrected amplitude from PKE solution [2].

*2.3 Exponential Transform Method*

The ET method was designed to enhance accuracy of the conventional theta method [4]. This method anticipates exponential variation of the neutron flux. Similar with quasi-static methods, the regional flux is factorized into two components in ET method:

$$\phi(\mathbf{r}, E, t) = e^{\alpha(\mathbf{r}, E)t} \tilde{\phi}(\mathbf{r}, E, t). \qquad (10)$$

The transformed flux $\tilde{\phi}(\mathbf{r}, E, t)$ will vary slowly when neutron flux changes exponentially. Introducing Eq. (10) into Eq. (1) yields equation similar with Eq. (4):

$$\frac{1}{v_g^m} \frac{d\tilde{\phi}_g^m}{dt} = e^{-\alpha_g^m t} \left[ (\mathbf{F} - \mathbf{F}_d - \mathbf{M})\Phi_g^m + S_{dg}^m - \frac{\alpha_g^m}{v_g^m} \phi_g^m \right]. \quad (11)$$

Eq. (11) is presented in discretized multi-group form for simplicity where subscript 'm' denotes region index and 'g' denotes energy group index. Similar with IQS the transformed flux is computed directly by solving Eq. (11). The difference of this method from quasi-static method is that exponential function in ET has regional and energy dependency while amplitude in quasi-static method has only time dependency. The main focus of this method is make the transformed flux less variable over time for small truncation error while IQS focused to find out the unique factorization of shape and amplitude based on exact perturbation theory.

**3. Application in nTRACER**

The transport solution in nTRACER is composed of 3 components: radial 2D method of characteristics (MOC), 3D coarse mesh finite difference (CMFD), and 1D axial MOC. These three components form the nonlinear system and it is solved in Picard iteration manner. Since there is already nonlinear iteration procedure in

transient solution algorithm of nTRACER, the nonlinear iteration of IQS can be straightforwardly incorporated by adding PKE solution procedure into the nonlinear iteration. The PCQS capability can be incorporated by adding corrector step that uses PKE solution before proceed to next time-step. The flowcharts for quasi-static capabilities are shown in Fig. 1. The neutron transport solver of nTRACER solves Eq. (4) rather than Eq. (1) in IQS algorithm. For IQS algorithm, two types of algorithm are implemented. First type uses the shape computed from solution of Eq. (4) while second type rescales the evaluated shape to preserve the constraint condition of flux factorization. In order to distinguish these algorithms, the first one is named as 'IQS' and the second one is named as 'IQS-rescale'. The ET method follows the same calculation flow of IQS algorithm in Fig. 1. Instead of solution of PKE, the inverse period are computed from adjacent neutron fluxes at 'PKE solve' stage.
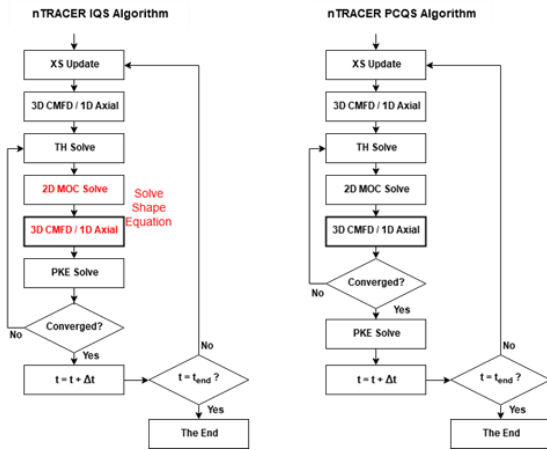


Fig. 1. Flowchart for quasi-static capabilities in nTRACER

## 3. Calculation Results

### 3.1 C5G7-TD Benchmark Results

The C5G7-TD is benchmark for solving the time-dependent multi-group neutron transport equation without feedback with sub-pin level heterogeneity. Detailed configuration of the core is presented in the reference [5]. The first sub-problem in the TD2 problem set (TD2-1) was used to investigate effectiveness of the quasi-static approaches as pure neutronics solver. TD2-1 is 2D problem that approximates the control rod transient as a ramp change of the material composition. The reference solution is generated with Backward Euler (BE) method with 1 ms time-steps. The micro time-step size for PKE solution is also set as 1 ms for this problem. The computing time for reference solution was 3588 seconds.

TD2-1 problem is solved with all possible methods with 50 ms time-steps and the results are listed in Table

1. With same time-step size, quasi-static approaches show better accuracy than BE. However, maximum error of ET remained in the 0.3% range, while other methods were within 0.1%. The power behavior of IQS-rescale resembles that of PCQS, rather than IQS as shown in Fig. 2. This is because the rescale of the shape function can be seen as the amplitude determination in PCQS algorithm with evaluated neutron flux. The average number of outer and inner iteration are also shown in Table 1. The outer iteration represents the entire procedure of the transient calculation including the 2D MOC. The computing time is determined by the number of outer iteration because 2D MOC solution has heavier computational cost than other components. The inner iteration means the number of iteration required by the linear system solver in 3D CMFD solve. IQS methods shows large discrepancy, which is larger than 10, with other methods for the inner iteration number. IQS-rescale decreases inner iteration number unlike IQS. On the contrary, when see the average number of outer iteration, all methods shows similar value. IQS shows the maximum discrepancy with BE but less than 0.2. As a result, all methods showed similar computing.

Table I: Results of C5G7 TD2-1 with 50 ms time-steps

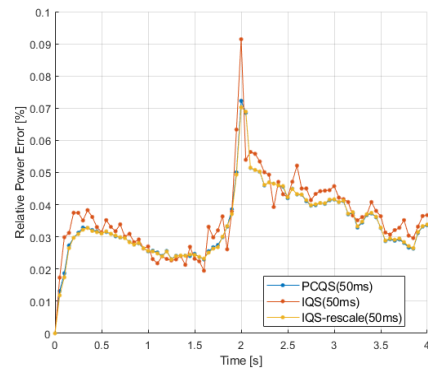| | BE | ET | PCQS | IQS | IQS-rescale |
|---|---|---|---|---|---|
| *Avg. Error (%)* | 0.062 | 0.045 | 0.034 | 0.036 | 0.034 |
| *Max. Error (%)* | 0.550 | 0.332 | 0.072 | 0.091 | 0.070 |
| *Avg, Outer Iter.* | 2.49 | 2.50 | 2.50 | 2.69 | 2.49 |
| *Avg. Inner Iter.* | 44.6 | 44.0 | 44.2 | 58.3 | 33.3 |
| *Time [s]* | 93.9 | 96.1 | 100.4 | 108.6 | 98.5 |



Fig. 2. Relative power error of quasi-static methods

### 3.2 SPERT III E-core Results

The Special Power Excursion Reactor Test (SPERT) is a series of experiments to obtain data for the reactivity accident [6]. The SPERT III E-core has characteristics of PWR and it is used as the benchmark for validation of dynamics calculation system. The efficiency of quasi-static approaches coupled with TH feedback is assessed with rod ejection from HZP power condition in SPERT III E-core. The initial power and

inlet temperature of test problem is $5\times10^{-5}$ MW and 260 °C, respectively. From the critical state, the reactivity was inserted by ejection of transient control rod and the inserted amount was 1.19$. For TH solve, a simplified closed pin channel T/H model composed of 1D axial heat convection and a radial heat conduction was used. Reference solution was generated by BE method with 1 ms time-steps. It takes 11 hours 50 minutes to generate the reference solution. Again, the same time-step size as the reference time-step size was used as the micro time-step size for PKE solution in quasi-static methods.

Table II: Results of SPERT III E-core with 5 ms time-steps

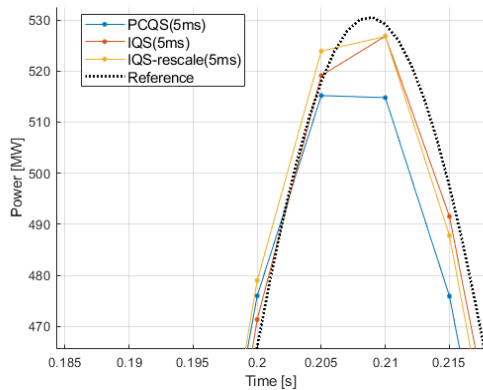|  | BE | ET | PCQS | IQS | IQS-rescale |
|---|---|---|---|---|---|
| *Max. Error (MW)* | 430.5 | 119.8 | 24.6 | 7.45 | 18.4 |
| *Avg, Outer Iter.* | 2.53 | 2.36 | 2.30 | 4.28 | 2.25 |
| *Avg. Inner Iter.* | 874.7 | 809.2 | 813.9 | 1517.8 | 743.1 |
| *Time [min]* | 179 | 171 | 166 | 287 | 181 |



Fig. 3. Power curve at the peak power region

The results of quasi-static approachess with 5 ms time-step size are compared with the reference solution and the results are listed in Table II. The solution generated with BE shows significantly forward shifted solution and it causes power error over 400 MW. The ET solution shows relatively less shifted solution than BE but it shows large error over 100 MW.

Inclusion of TH solve made several difference with C5G7-TD results. First, IQS methods shows better accuracy than PCQS because PCQS is not directly coupled with TH solver. Fig. 3 shows power behavior near peak power. PCQS solution shows 12 MW lower power than IQS methods. Because the fuel temperature rapidly changes at the peak power region, TH condition determined at predictor step of PCQS was not accurate enough. Second, large discrepancies was observed in outer iteration number between methods. Though IQS showed the best accuracy, it showed about 2 larger average outer iteration number. It led to an increase in calculation time of 100 minutes. On the other hand,

IQS-rescale shows a kind of acceleration effect. It shows the smallest value in both outer and inner iteration but discrepancy with other method (except IQS) was within 0.3 and showed not meaningful effect in computing time.

## 4. Conclusions

The quasi-static capabilities were implemented into the whole core transport transient calculation of nTRACER. The effectiveness of quasi-static methods is demonstrated with C5G7-TD benchmark analysis and rod ejection transient simulation in SPERT III E-core. From the SPERT III E-core analysis, IQS with shape rescaling was most efficient for nTRACER in terms of the overall efficiency and accuracy.

Further investigation with more sophisticated models for quasi-static methods like newton algorithms for nonlinear solution, coupling with high-order temporal discretization methods and improved coupling methods for TH feedback can be done as extension to the work here.

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