Real Variance Estimation in Monte Carlo Wielandt Calculaitons

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- **Based on the presentation at PHYSOR'08 Interlaken, Switzland**
- **Another Ref.:**
  Hyung Jin Shim and Chang Hyo Kim, "Tally Efficiency Analysis for Monte Carlo Wielandt Method," *Ann. Nucl. Eng.*, 36, 1694-1701 (2009).

Objectives of This Study

- Recently, the **Monte Carlo (MC) Wielandt method** for the eigenvalue calculations was proposed **to accelerate fission source convergence**.[1]

  ([1] T. Yamamoto and Y. Miyoshi, "Reliable Method for Fission Source Convergence of Monte Carlo Criticality Calculation with Wielandt's Method," *J. Nucl. Sci. Technol.* **41**, No. 2, pp. 99~107 (2004).)

- And it was reported that this method has **the potential to eliminate most of the underprediction bias** in confidence intervals for MC eigenvalue calculations.[2]

  ([2] F. Brown, "Wielandt Acceleration for MCNP5 Monte Carlo Eigenvalue Calculations," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007), Monterey, CA, April 15-19 (2007).)

- **However, the variance bias or the calculation efficiency using the real variance was not quantitatively evaluated for the MC Wielandt calculations.**

- **The objectives of this paper are**

  - to develop a real variance estimation method for the MC Wielandt calculations and

  - to analyze the efficiency of the MC Wielandt method by the FOM based on the real variance.

Approaches

- We have ever developed a real variance estimation method by using the inter-cycle correlations of the fission source distribution (FSD) for the conventional MC eigenvalue calculations. [3]

  ([3] Hyung Jin Shim and Chang Hyo Kim, "Real Variance Estimation Using an Inter-Cycle Fission Source Correlation for Monte Carlo Eigenvalue Calculations," *Nucl. Sci. Eng.*, 162, 98-108 (2009).)

- **And we found that this method can be readily applicable to the MC Wielandt calculations, even in MC runs with the small number of active cycles.**

- The presentation contents are
  1. introduction to the real variance estimation method using the FSD's inter-cycle covariance,
  2. derivation of the real variance for the MC Wielandt method,
  3. efficiency analysis of the MC Wielandt method for a very slow convergence problem.

Variance Bias

- Let us consider an MC eigenvalue calculation based on N active cycles with M neutron histories per cycle.
- Suppose that Q_j^i is the estimate of a tally Q from the j-th neutron history at active cycle i.
- Then the sample variance of the tally mean, $\overline{Q}$, is calculated by

$$\sigma_S^2\left[\overline{Q}\right] = \frac{1}{NM(NM-1)} \sum_{i=1}^{N}\sum_{j=1}^{M}\left(Q_j^i - \overline{Q}\right)^2, \qquad \text{(1)}$$

$$\overline{Q} = \frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M} Q_j^i \quad \text{or} \quad \overline{Q} = \frac{1}{N}\sum_{i=1}^{N} Q^i, \quad Q^i = \frac{1}{M}\sum_{j=1}^{M} Q_j^i \qquad \text{(2)}$$

Q^i means the MC estimate of Q at active cycle i.

- **However, $\sigma_S^2\left[\overline{Q}\right]$ is quite different from its real variance for slow convergence problems or problems with dominance ratios very close to 1.**

$$\boxed{\sigma^2\left[\overline{Q}\right] = E\left[\sigma_S^2\left[\overline{Q}\right]\right] + '\mathit{Bias}'} \qquad \text{(3)}$$

$\sigma^2\left[\overline{Q}\right]$ denotes the real or true variance.

Derivation of Variance Bias

- The real or true variance of $\overline{Q}$ can be written as

$$\sigma^2\left[\overline{Q}\right]=E\left[\overline{Q}^2\right]-E\left[\overline{Q}\right]^2$$
$$=E\left[\left(\frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M}Q_j^i\right)^2\right]-E\left[\frac{1}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M}Q_j^i\right]^2$$
$$=\frac{1}{NM}\sigma^2\left[Q_j^i\right]+\frac{1}{(NM)^2}\sum_{i,j}\sum_{i',j'\neq i,j}\mathrm{cov}\left[Q_j^i,Q_{j'}^{i'}\right] \qquad (4)$$

- On the other hand, the apparent variance of Q is defined as the expected value of the sample variance.

$$\sigma_A^2\left[\overline{Q}\right]=E\left[\sigma_S^2\left[\overline{Q}\right]\right] \qquad (5)$$

- As Ueki et al. [4] derived the relation between the real variance and the apparent variance of the eigenvalue *k*, the variance bias of $\sigma_S^2\left[\overline{Q}\right]$ can be quantified as

$$\sigma^2\left[\overline{Q}\right]-\sigma_A^2\left[\overline{Q}\right]=\frac{1}{N(N-1/M)}\sum_{l=1}^{N-1}(N-l)\mathrm{cov}\left[Q^i,Q^{i+l}\right] \qquad (6)$$

([4] T. Ueki et al, “Error Estimations and Their Biases in Monte Carlo Eigenvalue Calculations,” *Nucl. Sci. Eng.*, **125**, 1 (1997).)

Relation Betw. FSD and Tally

- The tally Q is calculated by using the corresponding detector response in the MC simulation as follows:

$$Q = \mathbf{R}^Q S \qquad (7)$$

where

$$\mathbf{R}^Q S = \int dP\, R^Q(P) S(P) \qquad (8)$$

$$R^Q(P) \equiv \sum_{j=0}^{\infty} \int_{\chi} dP'' g(P'') \int dP' K_j(P' \to P'') T\left(P \to P'\right) \qquad (9)$$

$$P \equiv (\mathbf{r}, E, \mathbf{\Omega}),$$

$$g(P) = \text{response function for the tally } Q \text{ at } P,$$

$$K_0(P' \to P) = \delta(P' - P),$$

$$K_j(P' \to P) = \int dP_1 \cdots \int dP_{j-1} K(P_{j-1} \to P) \cdots K(P' \to P_1),$$

$$K(P' \to P) \equiv C(\mathbf{r}'; E', \mathbf{\Omega}' \to E, \mathbf{\Omega}) T(E, \mathbf{\Omega}; \mathbf{r}' \to \mathbf{r}) = \text{transport kernel}$$

$$S(P) = \text{fission source distribution.}$$

- ***$R^Q(P)$* means a *Q* contribution from the unit fission source generated at *P*.**

How to Quantify Tally's Inter-cycle Covariance

- Because a finite number of histories is simulated, $R^Q(P)$ and $S(P)$ in Eq. (8) cannot be measured in a continuous form. Therefore, one may divide the whole region into small nonoverlapping cells with a spatial volume, V_m $(m = 1, 2, \cdots, N_m)$, and define their cell-wise discrete functions.
- Then Eq. (7) can be described in a discrete from:

$$Q = \sum_m^{N_m} R_m^Q S_m \qquad \text{(10)}$$

$$S_m = \int_{V_m}\int_E\int_{\mathbf{\Omega}} S(\mathbf{r}, E, \mathbf{\Omega}) d\mathbf{r} dE d\mathbf{\Omega} = \int_{V_m} S(P)dP$$

$$R_m^Q = \int_{V_m} R^Q(P)S(P)dP \Big/ \int_{V_m} S(P)dP$$

- From the definition of covariance, tally's inter-cycle covariance can be written as

$$\mathrm{cov}\left[Q^i, Q^{i+l}\right] = E\left[\left(\sum_{m=1}^{N_m} R_m S_m^i - \sum_{m=1}^{N_m} R_m E\left[S_m\right]\right)\left(\sum_{m'=1}^{N_m} R_{m'} S_{m'}^{i+l} - \sum_{m'=1}^{N_m} R_{m'} E\left[S_{m'}\right]\right)\right]$$

$$= \sum_{m=1}^{N_m}\sum_{m'=1}^{N_m} R_m R_{m'} \,\mathrm{cov}\left[S_m^i, S_{m'}^{i+l}\right] \qquad \text{(11)}$$

How to Quantify FSD's Inter-cycle Covariance

- By the cycle-by-cycle error propagation model [5] and the direct posterior estimation method for the stochastic error's covariance [6], $\mathrm{cov}\left[S_m^i, S_{m'}^{i+l}\right]$ of Eq. (11) can be expressed as

$$\mathrm{cov}\left[S_m^i, S_{m'}^{i+l}\right] = \sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^{i'} a_{m'n'}^{i'+l}\,\mathrm{cov}\left[\varepsilon_n, \varepsilon_{n'}\right]$$

$$= \frac{1}{M}\sum_{i'=0}^{\infty}\sum_{n=1}^{N_m}\sum_{n'=1}^{N_m} a_{mn}^{i'} a_{m'n'}^{i'+l}\,\mathrm{cov}\left[\varepsilon_{n,j}, \varepsilon_{n',j}\right] \qquad (12)$$

$$\mathrm{cov}\left[\varepsilon_{n,j}, \varepsilon_{n',j}\right] = E\left[\left(S_{n,j}^i - E\left[S_n^i \middle| \mathbf{S}^{i-1}\right]\right)\cdot\left(S_{n',j}^i - E\left[S_{n'}^i \middle| \mathbf{S}^{i-1}\right]\right)\right] \qquad (13)$$

a_{mn}^j is m-th row and n-th column element of the matrix $\mathbf{A}^j$ and the matrix $\mathbf{A}$ is defined by

$$\mathbf{A} = \frac{1}{k_0}\left(\mathbf{H} - \mathbf{S}_0 \cdot \boldsymbol{\tau}^T \cdot \mathbf{H}\right), \qquad (14)$$

$\tau = N_m$ dimensional row vector $(1,1,\cdots,1)$, $\mathbf{H}$ = fission matrix,

$\mathbf{S_0}$ = main mode fission source distribution, k_0 = main mode eigenvalue.

([5] E. M. Gelbard and R. E. Prael, "Monte Carlo Work at Argonne National Laboratory, ANL-75-2(NEACRP-L-118) (1974).

([6] H. J. Shim and C. H. Kim, "Stopping Criteria of Inactive Cycle Monte Carlo Calculations," *Nucl. Sci. Eng.*, **157**, pp.132-141 (2007).)

Transport Equation

- The time-independent Boltzmann transport equation for neutrons can be written in operator notation as

$$\mathbf{T}\psi = \frac{1}{k}\mathbf{F}\psi \qquad (15)$$

where

$$\mathbf{T}\psi = \left[\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\psi(\mathbf{r},E,\mathbf{\Omega}) - \int dE'\int d\mathbf{\Omega}'\Sigma_s(\mathbf{r};E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega})\psi(\mathbf{r},E',\mathbf{\Omega}') \qquad (16)$$

$$\mathbf{F}\psi = \frac{\chi(E)}{4\pi}\int dE'\int d\mathbf{\Omega}'\nu(E')\Sigma_f(\mathbf{r},E')\psi(\mathbf{r},E',\mathbf{\Omega}') \qquad (17)$$

$\Sigma_t(\mathbf{r},E) =$ total cross section

$\Sigma_s(\mathbf{r};E',\mathbf{\Omega}'\rightarrow E,\mathbf{\Omega}) =$ scattering cross section from $E',\mathbf{\Omega}'$ to $E,\mathbf{\Omega}$

$\chi(E) =$ fission spectrum

$\nu(E') =$ mean number of fission neutrons produced in a fission

$\Sigma_f(\mathbf{r},E') =$ fission cross section

$k =$ mutiplication factor

Conventional MC Power Method

- By inverting **T** and operating with **F** on both sides of Eq. (15), we obtain the following form

$$\mathbf{F}\psi = \frac{1}{k}\left[\mathbf{F}\mathbf{T}^{-1}\right]\mathbf{F}\psi \quad \cdots\cdots \quad (18)$$

- And the FSD, S and fission operator, **H** are defined as follows

$$S = \mathbf{F}\psi \quad \cdots\cdots \quad (19)$$

$$\mathbf{H} = \mathbf{F}\mathbf{T}^{-1} \quad \cdots\cdots \quad (20)$$

- The fission operator $\mathbf{H}(\mathbf{r}', E', \mathbf{\Omega}' \to \mathbf{r}, E, \mathbf{\Omega})$ denotes the number of first-generation fission neutrons born per unit volume about $(\mathbf{r}, E, \mathbf{\Omega})$, due to a parent neutron born per unit volume at $(\mathbf{r}', E', \mathbf{\Omega}')$.
- Inserting Eqs. (19) and (20) into Eq. (18) leads the following eigenvalue equation

$$S = \frac{1}{k}\mathbf{H}S \quad \cdots\cdots \quad (21)$$

- In the conventional MC eigenvalue calculations, the FSD is iteratively updated as

$$S^{i} = \frac{1}{k^{i-1}}\mathbf{H}S^{i-1} + \varepsilon^{i} \quad \cdots\cdots \quad (22)$$

MC Wielandt Method

- The Wielandt method is characterized by rewriting Eq. (15) as

$$\mathbf{T}\psi - \frac{1}{k_e}\mathbf{F}\psi = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{F}\psi \qquad (23)$$

k_e is an estimated eigenvalue.

- By inverting $\left(\mathbf{T} - \mathbf{F}/k_e\right)$ and operating with $\mathbf{F}$ on both sides of Eq. (23), we obtain the following equation

$$\mathbf{F}\psi = \left(\frac{1}{k} - \frac{1}{k_e}\right)\left[\mathbf{F}\left(\mathbf{M} - \frac{1}{k_e}\mathbf{F}\right)^{-1}\right]\mathbf{F}\psi \qquad (24)$$

- Inserting Eq. (19) into Eq. (24) leads the following eigenvalue equation

$$S = \left(\frac{1}{k} - \frac{1}{k_e}\right)\mathbf{H}'S \qquad (25) \qquad\qquad \mathbf{H}' = \mathbf{F}\left(\mathbf{M} - \frac{1}{k_e}\mathbf{F}\right)^{-1} \qquad (26)$$

- Applying the power method to Eq. (25), the FSD is updated iteratively in the Wielandt method as

$$S^i = \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}'S^{i-1} + \varepsilon^i \qquad (27)$$

Algorithm for MC Wielandt Method (1/2)

- Using Eq. (20), the fission operator $\mathbf{H}'$ in the Wielandt's method can be expressed as

$$\mathbf{H}' = \mathbf{F}\left[\mathbf{M} - \frac{1}{k_e}\mathbf{F}\right]^{-1} = \mathbf{F}\left[\mathbf{M} - \frac{1}{k_e}\mathbf{H}\mathbf{M}\right]^{-1} = \mathbf{F}\left[\left(\mathbf{I} - \frac{\mathbf{H}}{k_e}\right)\mathbf{M}\right]^{-1} = \mathbf{F}\mathbf{M}^{-1}\left(\mathbf{I} - \frac{\mathbf{H}}{k_e}\right)^{-1}$$
$$= \mathbf{H}\left(\mathbf{I} - \frac{\mathbf{H}}{k_e}\right)^{-1} \qquad \text{(28)}$$

- By the Taylor's series expansion, $\left(\mathbf{I} - \mathbf{H}/k_e\right)^{-1}$ in Eq. (28) can be written as

$$\left(1 - \frac{\mathbf{H}}{k_e}\right)^{-1} = 1 + \frac{\mathbf{H}}{k_e} + \left(\frac{\mathbf{H}}{k_e}\right)^2 + \cdots \qquad \text{(29)}$$

- Inserting Eq. (29) into Eq. (28) leads to

$$\mathbf{H}' = \mathbf{H}\left(1 + \frac{\mathbf{H}}{k_e} + \left(\frac{\mathbf{H}}{k_e}\right)^2 + \cdots\right) \qquad \text{(30)}$$

Algorithm for MC Wielandt Method (2/2)

- Substitution of Eq. (30) into Eq. (27) leads

$$S^i = \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}S^{i-1} + \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}\left(\left(\frac{\mathbf{H}}{k_e}\right)S^{i-1}\right) + \left(\frac{1}{k^{i-1}} - \frac{1}{k_e}\right)\mathbf{H}\left(\left(\frac{\mathbf{H}}{k_e}\right)^2 S^{i-1}\right) + \cdots + \varepsilon^i \quad \text{(31)}$$

- The first term in the RHS of Eq. (31) means the number of first next-cycle fission sites generated from S^{i-1}. From comparing this term with the RHS of Eq. (22), one can see that it is less by as much as $\mathbf{H}S^{i-1}/k_e$. And these fission sources of $\mathbf{H}S^{i-1}/k_e$ generate the second next-cycle fission sites as much as the second term in the RHS of Eq. (31).
- In the same way, the next-cycle fission sites from all the generations are sampled. This process is exactly the same as the algorithm described in Ref. [1].

([1] T. Yamamoto and Y. Miyoshi, "Reliable Method for Fission Source Convergence of Monte Carlo Criticality Calculation with Wielandt's Method," J. Nucl. Sci. Technol., v. 41, n. 2, pp. 99~107 (2004).)

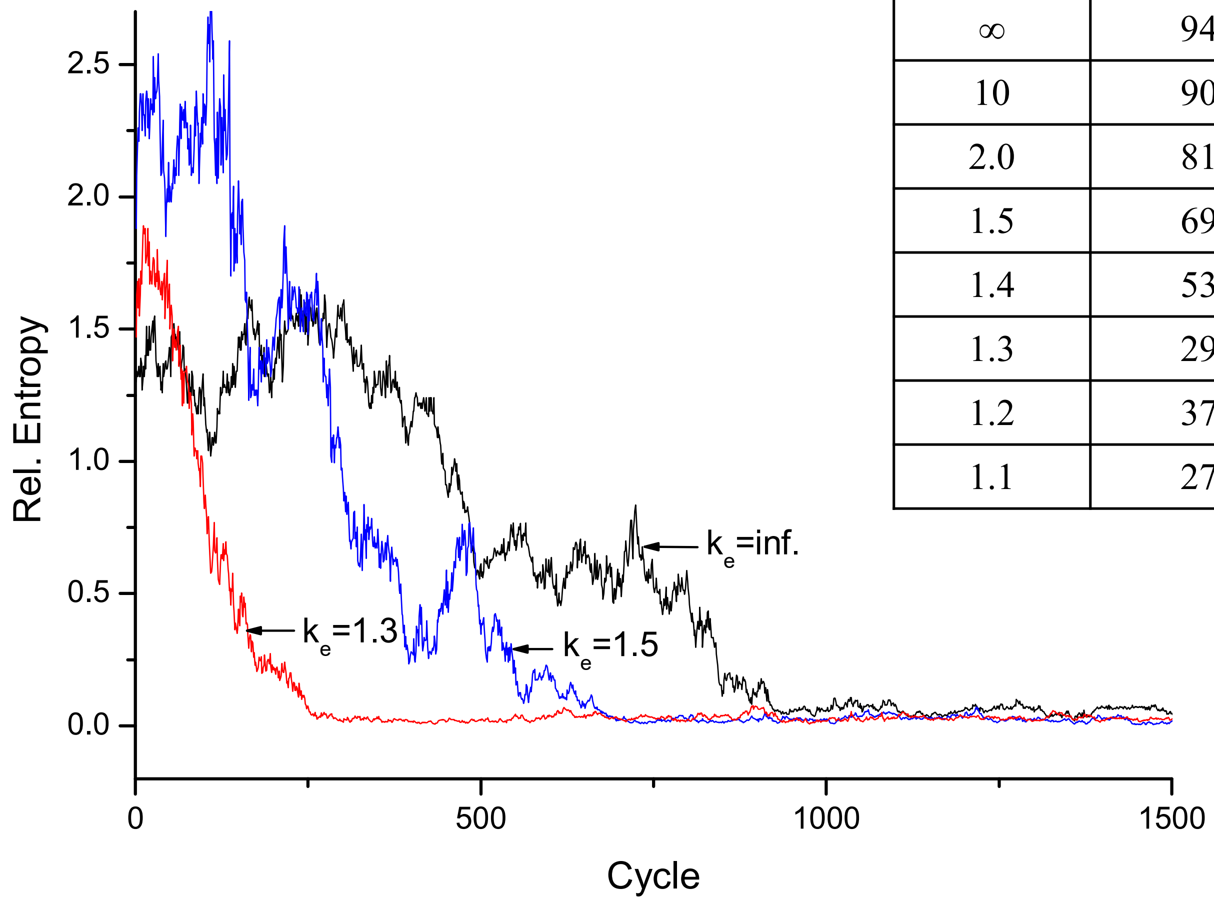
Real Variance Estimation In MC Wielandt Calculations

- The sample variance of a tallied nuclear parameter or a tally in the MC Wielandt calculations must be biased because of inter-cycle correlations of FSD by Eq. (27).
- From comparing Eq. (27) with Eq. (22), we can see that the only difference is the change from the operator **H** into **H'**.
- Therefore the real variance estimation method using FSD's inter-cycle correlation can be directly applied to the MC Wielandt calculations by changing **H** into **H'**.

Results of Source Convergence

- Cycle number of the fission source convergence were diagonized by the Ueki's posterior method.

k_e	convergence cycle	required time (min.)
∞	944	57.4
10	907	61.8
2.0	810	109.9
1.5	695	142.9
1.4	538	127.5
1.3	293	83.7
1.2	373	135.4
1.1	277	143.2



Application Results of the IAEA Source Conv. Problem #1 (10,000 histories X 1,000 active cycles)

k_e	CPU Time (min.)	power	sample variance		estimated real variance	
			R	FOM	R	FOM
(1,3) Assembly						
∞	128	5.38E-04	0.00080	12204.17	0.10200	0.75
10.0	142	6.42E-04	0.00073	13186.95	0.05566	2.27
2.0	279	6.36E-04	0.00070	7318.43	0.04230	2.00
1.5	421	6.41E-04	0.00073	4456.24	0.03673	1.76
1.4	484	6.34E-04	0.00075	3676.01	0.03411	1.78
1.3	581	6.54E-04	0.00076	2979.90	0.02930	2.01
1.2	734	6.54E-04	0.00081	2075.54	0.02801	1.74
1.1	1046	6.46E-04	0.00094	1081.90	0.02160	2.05
(3,3) Assembly						
∞	128	1.55E-04	0.00158	3128.77	0.08420	1.10
10.0	142	1.85E-04	0.00144	3388.95	0.07174	1.37
2.0	279	1.65E-04	0.00145	1705.60	0.05005	1.43
1.5	421	1.66E-04	0.00150	1055.44	0.03806	1.64
1.4	484	1.70E-04	0.00151	906.87	0.03629	1.57
1.3	581	1.56E-04	0.00162	655.84	0.03281	1.60
1.2	734	1.52E-04	0.00171	465.70	0.02878	1.64
1.1	1046	1.64E-04	0.00183	285.46	0.02301	1.81

Application Results of the IAEA Source Conv. Problem #1 (100,000 histories X 1,000 active cycles)

k_e	CPU Time (min.)	power	sample variance		estimated real variance	
			R	FOM	*R*	FOM
(1,3) Assembly						
∞	1253	6.41E-04	0.00023	15082.05	0.02034	1.93
10.0	1395	6.56E-04	0.00023	13548.18	0.01803	2.20
2.0	2774	6.65E-04	0.00021	8174.50	0.01251	2.30
1.5	4215	6.62E-04	0.00023	4484.60	0.01055	2.13
1.4	4859	6.61E-04	0.00023	3890.80	0.00963	2.22
1.3	5824	6.57E-04	0.00024	2981.21	0.00900	2.12
1.2	7430	6.50E-04	0.00026	1991.06	0.00815	2.03
1.1	10591	6.55E-04	0.00029	1122.66	0.00680	2.04
(3,3) Assembly						
∞	1253	1.59E-04	0.00049	3322.95	0.02374	1.42
10.0	1395	1.62E-04	0.00049	2985.00	0.02194	1.49
2.0	2774	1.61E-04	0.00047	1631.94	0.01523	1.55
1.5	4215	1.61E-04	0.00048	1029.67	0.01231	1.57
1.4	4859	1.59E-04	0.00049	857.24	0.01139	1.59
1.3	5824	1.60E-04	0.00050	686.87	0.01030	1.62
1.2	7430	1.61E-04	0.00053	479.16	0.00902	1.65
1.1	10591	1.62E-04	0.00058	280.67	0.00741	1.72

Conclusion

- A variance-bias estimation method using an inter-cycle FSD's correlation in the conventional MC eigenvalue calculations is applied to the MC Wielandt calculations.
- **From the FOM's based on the estimated real variance for the slow-convergence benchmark problem, it was shown that the tally efficiency is enhanced by the MC Wielandt calculations.**