Single-Precision Calculation of Iterative Refinement of Eigenpairs of a Real Symmetric-Definite Generalized Eigenproblem by Using a Filter Composed of a Single Resolvent

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- **By using a filter, we solve eigenpairs of a real symmetric-definite GEVP whose eigenvalues are in a specified interval.**
- **The system of linear equations to give the action of a resolvent used in the filter is solved by some direct method.**
- **To reduce both costs to factor the matrix and to store the factors, the filter we used is a polynomial of a single resolvent.**

  Such a filter does not have a good shape in the transfer function, and the residuals of the approximate eigenpairs will not be small.
- **We iterated the combination of orthonormalization and filtering a few times to improve the approximate eigenpairs.**

Filters Composed of a Single Resolvent

- **Eigenpairs of a real symmetric-definite GEVP $A\,v = \lambda B\,v$ is approximated whose eigenvalues are in the specified interval $[\,a,\,b\,]$ by using a filter.**

- **A filter is composed of resolvents $\mathcal{R}(\rho_i) \equiv (A - \rho_i B)^{-1}B$, here shifts ρ_i are complex numbers.**

  An application of the resolvent $y \leftarrow \mathcal{R}(\rho)\,x$ reduces to solve $C(\rho)\,y = B\,x$ for y whose coefficient $C(\rho)$ is $A - \rho B$. In this study, some direct method is used to solve it.

- **The shifted matrix $C(\rho)$ is real-symmetric when ρ is real, and is also positive-definite when ρ is less than the minimum eigenvalue.**

- **When ρ is imaginary, $C(\rho)$ is complex-symmetric and non-singular.**

- **The system of symmetric linear equations is solved by the modified Cholesky LDL^T decomposition and forward/backward substitutions.**

- **When a system of linear equations of a large size is solved by some direct method, there are following computational bottlenecks :**
  - **The amount of *computation* for matrix decompositions**
  - **The amount of *storage* to hold factors of matrices**

  To reduce these amounts especially the amount of storage, in this study we minimized the number of resolvents that compose the filter to only one.

- **Two types of filters composed of only a single resolvent:**

$$\mathbf{1)}\ \mathcal{F} = g_{\mathsf{s}}\, T_n\big(\, 2\,\gamma\, \mathcal{R}(\rho) - I\,\big)\,,$$

$$\mathbf{2)}\ \mathcal{F} = g_{\mathsf{s}}\, T_n\big(\, 2\,\gamma'\, \mathrm{Im}\, \mathcal{R}(\rho') - I\,\big)\,.$$

  - **For type-1, the shift** ρ **is real, and the eigenvalue interval** $[\,a,\, b\,]$ **must be at the lower-end.**
  - **For type-2, the shift** ρ' **is an imaginary, and the interval may be located anywhere.**

Here, g_{s} **is the upper-bound of the filter's transfer function magnitude in the stop-band, and** γ **and** γ' **are real constants, and** I **is the identity operator.**

- **Filters composed of only a single resolvent cannot have good shapes in their transfer functions.**
  - **Transfer functions cannot make steep changes in value.** $\Rightarrow$ μ**, the ratio of the width of transition-bands to the width of the pass-band, cannot be made very small.**
  - **When** $g_{\mathbf{s}}$ **is set to a very small value, the** max-min **ratio of the transfer function in the pass-band** $\lambda \in [a, b]$ **will be large.**
  - **If this** max-min **ratio is very large, after the filtering the rates of required eigenvectors contained in the set of vectors tend to have different orders of magnitudes.**

– **By the filtering, in the set of vectors, those eigenvectors whose transfer-rates are large are enhanced, but those ones whose rates are smaller are diminished.**

⇒ In the filtered vectors, the information of eigenvectors with smaller transfer-rates tends to become less accurate.

⇒ Some of the approximate eigenpairs may not meet the required accuracy or may be missing.

⇒ Therefore, it may be necessary to improve the approximate eigenpairs obtained from a single filter application.

Iterative Refinement of Eigenpairs by Using a Filter

- **So far, we have assumed the filter is applied only once.**
- **Even the filter's transfer function is not good in shape, the approximate eigenpairs can be improved if the combination of orthonormalization and filtering is iterated a small number of `IT` times by the following procedure:**

1) Let Y be an initial set of m random vectors.

2) Iterate the followings IT times :

Y **is** B**-orthonormalized to obtain** X **;**
X **is filtered to obtain** Y **.**

3) Considering the shape of the transfer function, construct the required approximate eigenpairs from both X and Y.

- **In the iteration, m the number of vectors is updated to the effective rank which is determined by the B-orthonormalization.**

- **Orthonormalization for each iteration prevents the tendency of those eigenvectors with relatively small transfer-rates to reduce information by the filtering.**

  The principle of the method is well-known as the *orthogonal iteration.*

EXPERIMENTS

System Environment

- **Machine** : Oakforest-PACS (Fujitsu PRIMERGY CX1640M1)
- **CPU** : Intel Xeon Phi 7250 (KNL) (1.4 GHz, 68 Cores)
- **Theoretical Peak Performance** : 3.04 TFLOPS (D-P)
- **Memory:** 16 GiB MCDRAM + 96(82) GiB DDR4(2400 RDIMM 6ch)
  (Cache mode)
- **OS** : CentOS 7.6
- **Source Code** : Fortran 90 + OpenMP directives
- **Compiler:** intel fortran version 19.0.5.281
- **Options** : "-fast -xMIC-AVX512 -qopenmp -align array64byte"
- **Number of Threads** : 204 (3 times of num of cores)
- **Thread Allocation:** "KMP_AFFINITY = balanced"

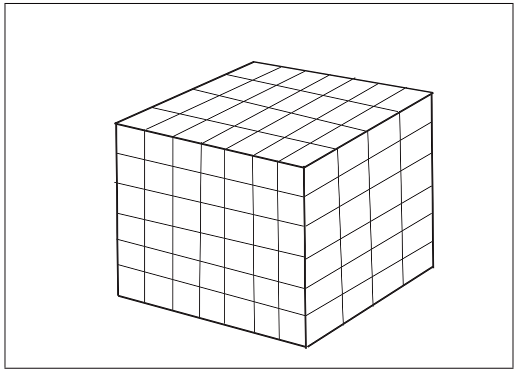
Test Problem

- **A 3-D Laplace eigenvalue problem with zero-Dirichlet boundary for a cubic region with a side length of π :**

$$-\Delta\,\Psi(x,y,z) = \lambda\,\Psi(x,y,z)\,. \tag{1}$$

By FEM discretization, a real symmetric definite GEVP is obtained : $\quad A\,v = \lambda B\,v$ **.**

- **Sides of the cube are equi-divided into $N_1{+}1$, $N_2{+}1$, $N_3{+}1$ sub-intervals to make finite elements.**



Concept of FE partitioning. For the Case $(N_1, N_2, N_3) = (3, 5, 6)$.

- **FEM basis : Tri-linear functions.**
- **Matrix size of** A **and** B **:** $N = N_1\, N_2\, N_3$ $(N_1 \leq N_2 \leq N_3\ )$ **.**
  Lower band-width of A **and** B **:** $w_L = 1 + N_1 + N_1\, N_2$ **.**
- **For this test problem, the exact eigenvalues can be calculated by simple expressions.**
  The number of eigenvalues in an arbitrary interval can be counted also.
- **By using a filter, we approximate all eigenpairs whose eigenvalues are in the interal** $[\,a,\ b\,]$**.**

Relative Residual of Approximate Eigenpair

- **The quality of an approximate eigenpair (λ, v) can be evaluated by the relative residual defined as :**

$$\Theta \;\equiv\; \frac{||\, A\, v - \lambda B\, v\, ||_2}{||\, \lambda B\, v\, ||_2}\,. \tag{2}$$

- **The approximate eigenpair is accurate if Θ is small.**
  - **Θ is independent from the normalization of vector v.**
  - **Θ is invariant if A and B are multiplied by a constant.**

- **When ϕ is the angle between two vectors $A\, v$ and $\lambda\, B\, v$, then the following holds :**

$$\sin\phi \;\leq\; \Theta\,. \tag{3}$$

Experiments of Iterative Refinements (in S-P)

FE partitionings of a cube : $(N_1,\ N_2,\ N_3) = (50,\ 60,\ 70)$**.**
A **and** B **have size** $N{=}210,000$ **and lower-bandwidth** $w_L{=}3,051$**.**

- **S-P (IEEE 754 FP32,** 7.2 **digits precision) is used for numbers and arithmetics.**

- **S-P has little margin for accuracy. However,**
  - **Recently, power saving through low-precision calculations has been attracting attention.**
  - **For some systems, S-P is much faster to calculate than D-P.**

Designs of Filters for Present Experiments

- **For lower-end eigenpairs, the filter is a deg n Chebyshev polynomial of a resolvent with a real shift.**
- **For interior eigenpairs, the filter is a deg n Cheby-poly of the imaginary-part of a resolvent with an imaginary shift.**
- **We specify the filter's transfer function by a set of three parameters (μ, $g_{\mathtt{s}}$, n).**
- **We prepared four filters with different settings to solve lower-end eigenpairs or interior eigenpairs.**
  - **Both $\mu = 1.5$ and $g_{\mathtt{s}}$ =1E-5 for all cases.**
  - **Degree n is set to 4, 6, 8 and 10.**
- **The values of $g_{\mathtt{p}}$ and $g_{\mathtt{s}} / g_{\mathtt{p}}$ are shown in the Table.**

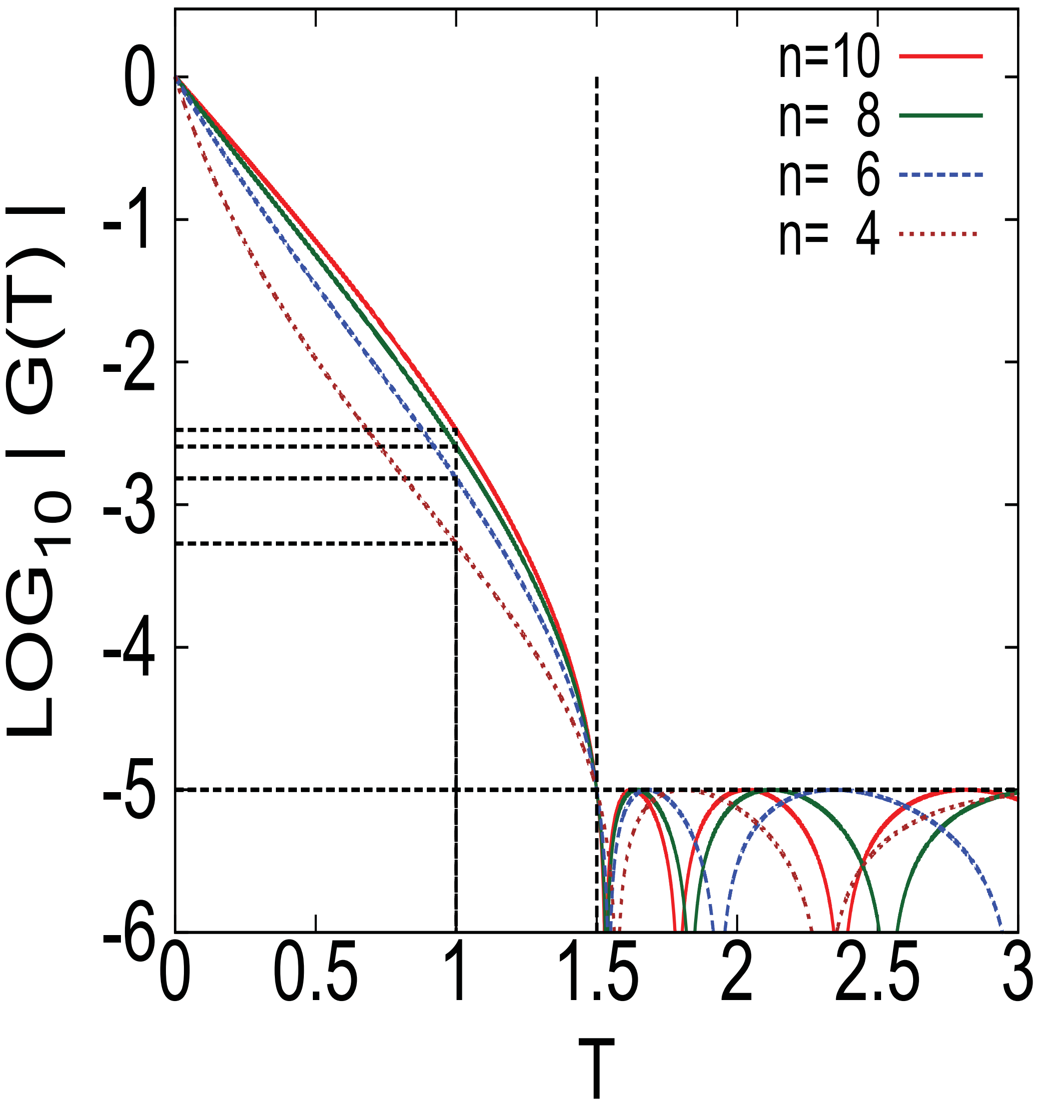
Settings and Properties of the Filters

			for lower-end eigenpairs		for interior eigenpairs	
μ	g_{s}	n	g_{p}	$g_{\mathrm{s}} / g_{\mathrm{p}}$	g_{p}	$g_{\mathrm{s}} / g_{\mathrm{p}}$
1.5	1E-5	4	5.3E-4	1.9E-2	3.7E-3	2.7E-3
1.5	1E-5	6	1.5E-3	6.5E-3	1.3E-2	8.0E-4
1.5	1E-5	8	2.6E-3	3.9E-3	2.1E-2	4.7E-4
1.5	1E-5	10	3.3E-3	3.0E-3	2.7E-2	3.7E-4

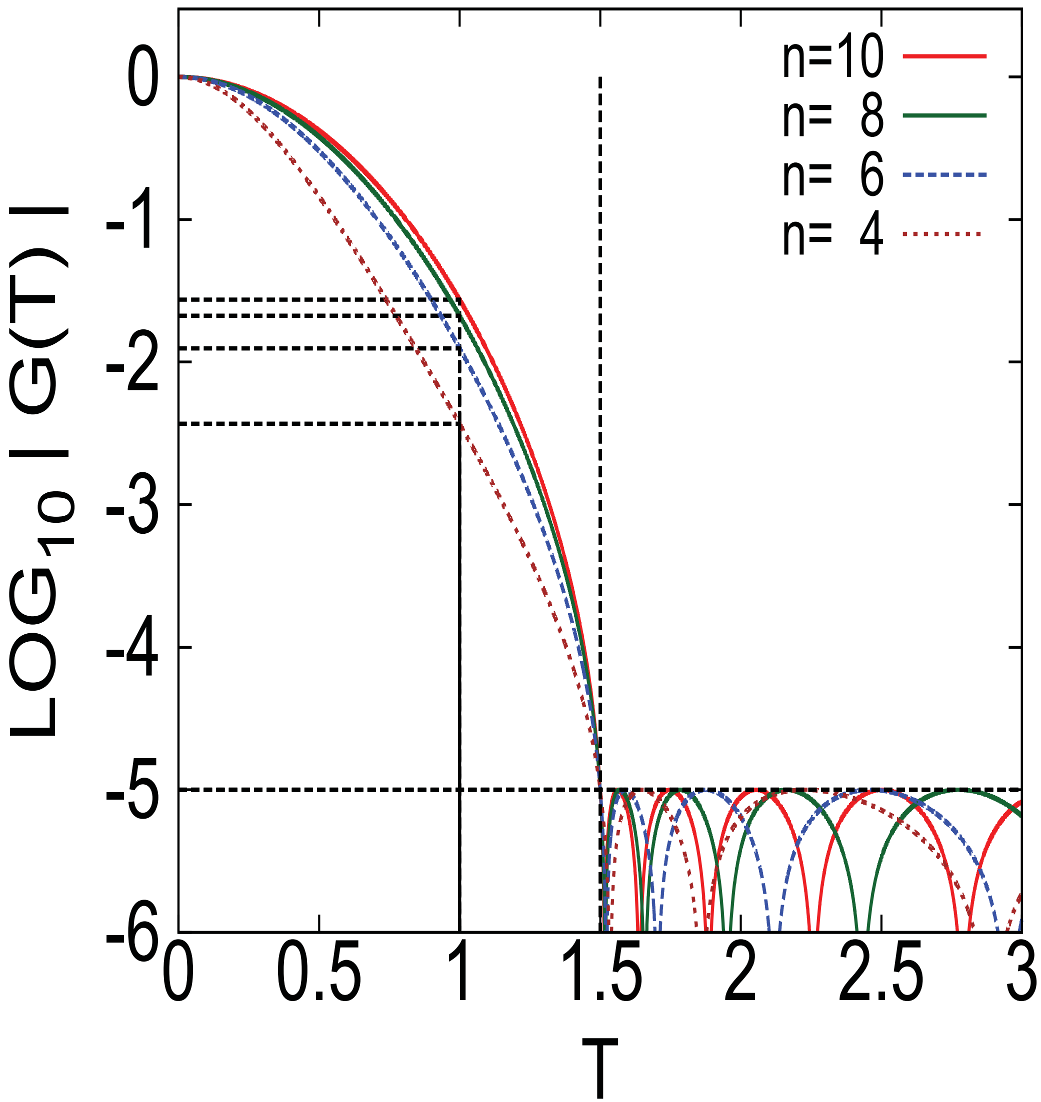
($g_{\mathrm{s}}/g_{\mathrm{p}}$ is rate of reduction per iteration.)

The larger the value of g_{p}, the better the filter property.
The smaller the value of $g_{\mathrm{s}}/g_{\mathrm{p}}$, the better the filter.

Transfer Function Magnitude $|g(t)|$ ($\mu = 1.5$, $g_s = \texttt{1E-5}$)



For lower-end eigenvalues



For interior eigenvalues (showing only the right-half)

The Shift of Resolvent of Each Filter

The shift of the resolvent is shown for each filter with parameters (μ=1.5, g_{s}=1E-5, n) to solve eigenpairs whose eigenvalues are either in the lower-end interval $[0, 100]$, or in the interior interval $[100, 200]$.

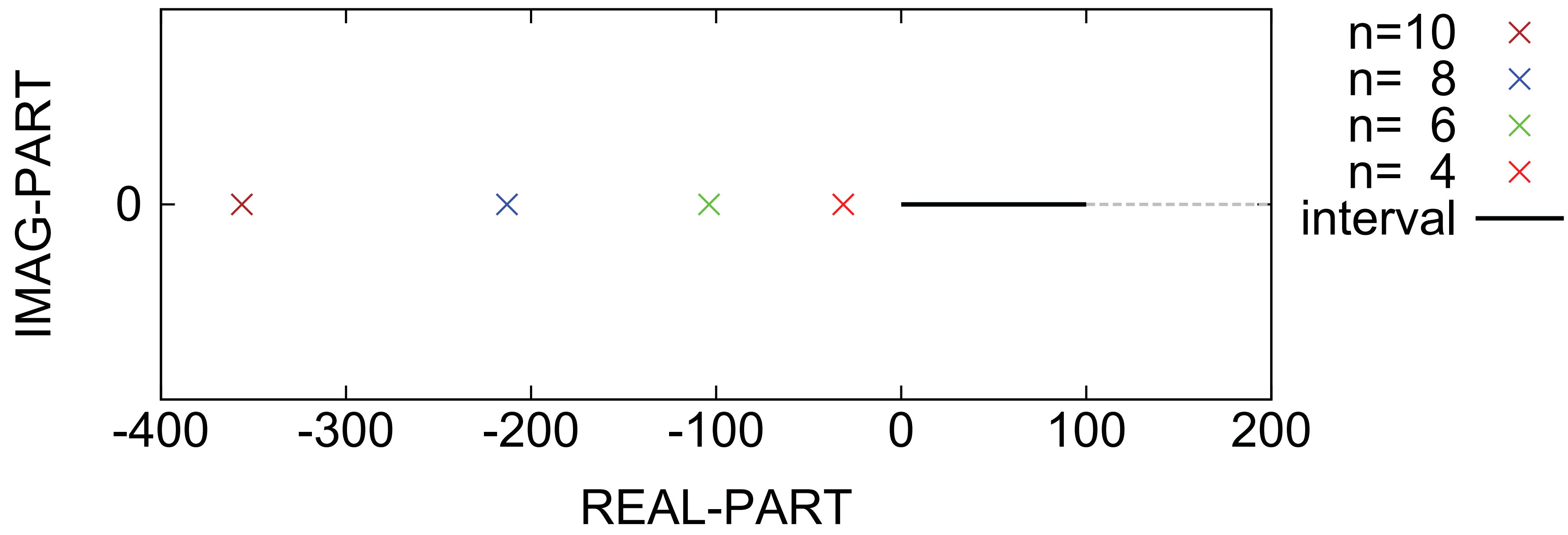
For lower-end eigenpairs

n	**real shift** ρ
4	-31.259
6	-103.842
8	-213.061
10	-356.232

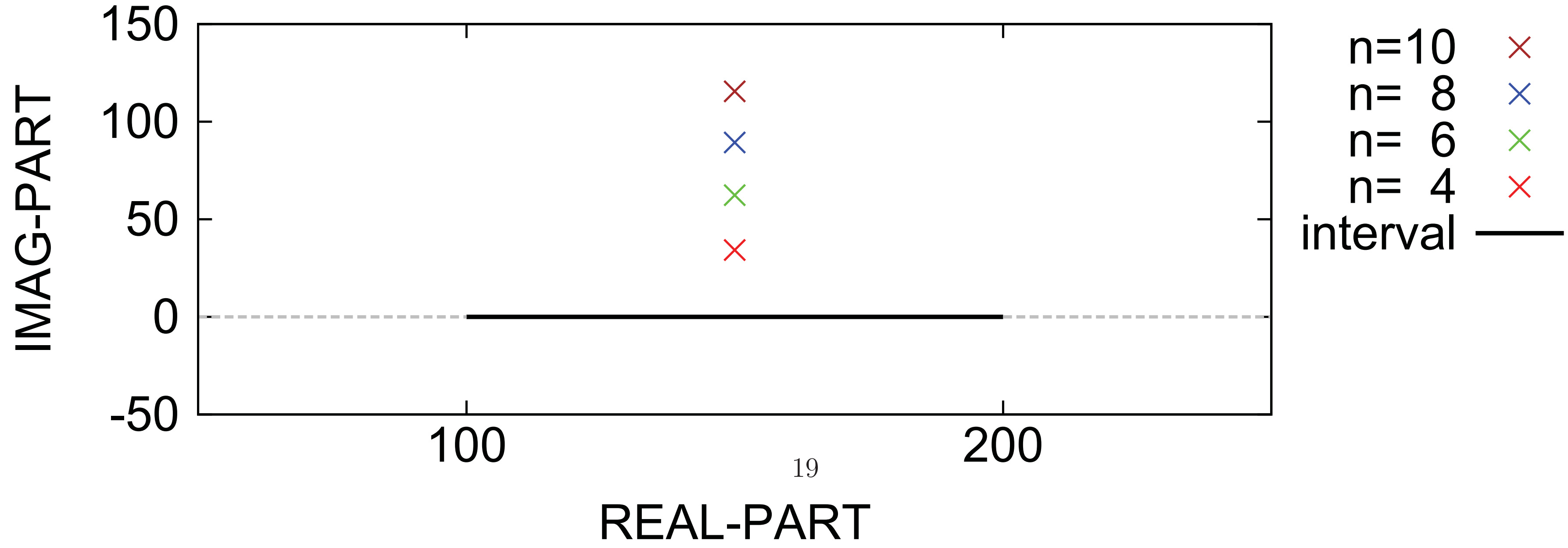
For interior eigenpairs

n	**imaginary shift** ρ'
4	$150 + 34.237\sqrt{-1}$
6	$150 + 62.403\sqrt{-1}$
8	$150 + 89.386\sqrt{-1}$
10	$150 + 115.580\sqrt{-1}$

The lower-end interval $[0, 100]$ and the real shift ρ



The interior interval $[100, 200]$ and the imaginary shift ρ'



Ex-1 : LOWER-END EIGENPAIRS

(Ex-1): Solution of Lower-end Eigenpairs

- **In the lower-end interval $[\,a,\ b\,] = [\,0,\ 100\,]$, there are 402 eigenpairs to be solved.**

- **The union of the pass-band and the transition-band $[\,a,\ b'\,] = [\,0,\ 150\,]$ contains 764 eigenvalues.**

- **The number of initial vectors used : $m = 800$. (More than 764 and would be sufficient.)**

- **The results of the experiment are shown.**

(Ex-1): Num of Approx Eigenpairs and Max Rel Residuals

($\mu = 1.5$, $g_{\mathtt{s}} = \mathtt{1E{-}5}$, $m = 800$, the correct num eigenpairs is 402).

$n = 4$

IT	# Eigenpairs	Max Rel Residual
1	139(139)	1.6E-01 (1.6E-01)
2	402(402)	2.7E-02 (2.8E-02)
3	402(402)	1.2E-03 (6.0E-04)
4	402(402)	3.5E-04 (1.2E-05)
5	402(402)	3.5E-04 (2.4E-07)
6	402(402)	3.5E-04 (4.4E-09)

$n = 6$

IT	# Eigenpairs	Max Rel Residual
1	222(221)	2.2E-01 (2.1E-01)
2	402(402)	1.0E-02 (1.2E-02)
3	402(402)	2.9E-04 (8.6E-05)
4	402(402)	2.9E-04 (5.7E-07)
5	402(402)	2.9E-04 (4.5E-09)
6	402(402)	2.9E-04 (2.8E-11)

$n = 8$

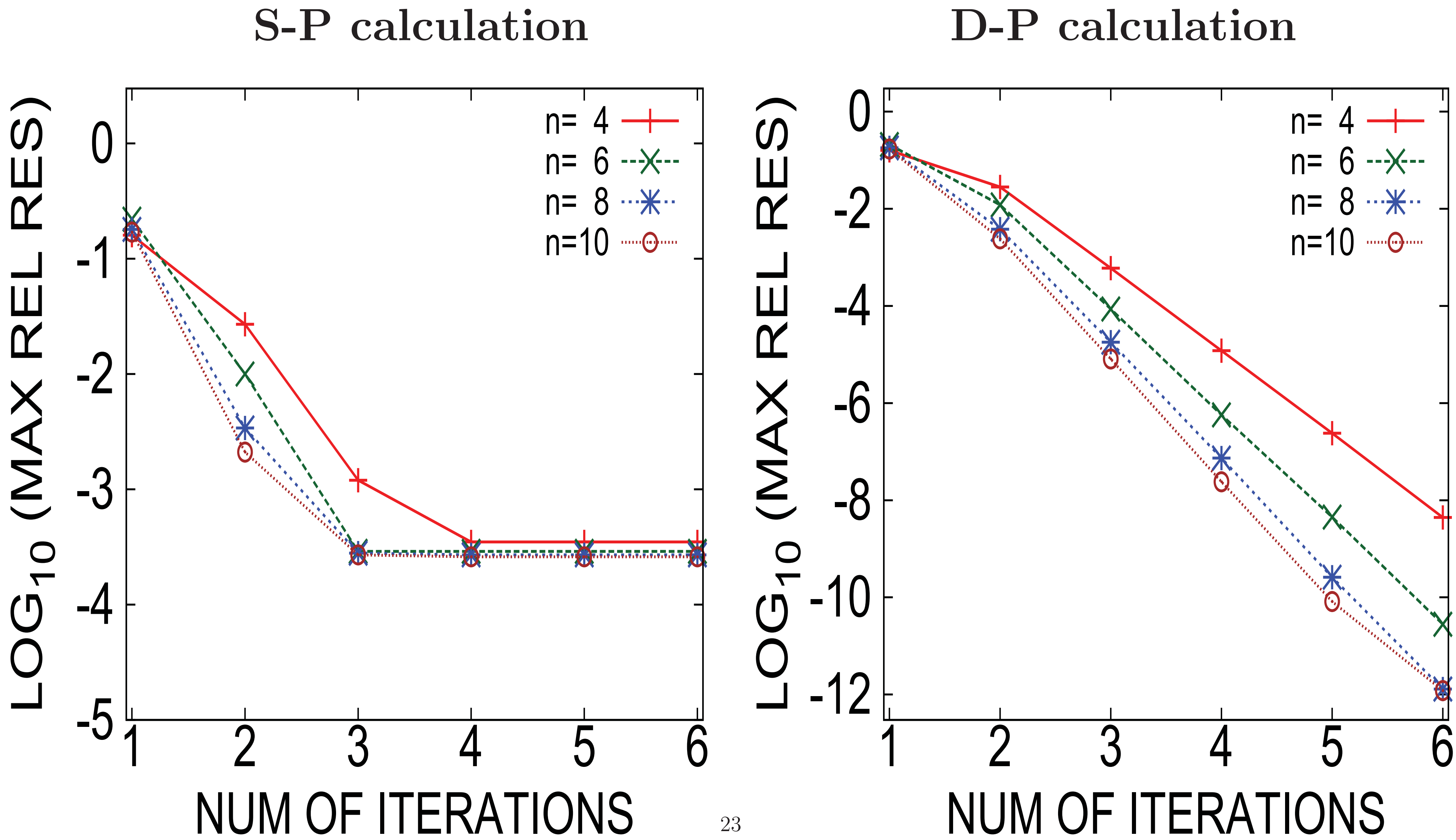
IT	# Eigenpairs	Max Rel Residual
1	265(265)	1.8E-01 (1.8E-01)
2	402(402)	3.4E-03 (3.8E-03)
3	402(402)	2.8E-04 (1.8E-05)
4	402(402)	2.7E-04 (7.4E-08)
5	402(402)	2.7E-04 (2.6E-10)
6	402(402)	2.7E-04 (1.3E-12)

$n = 10$

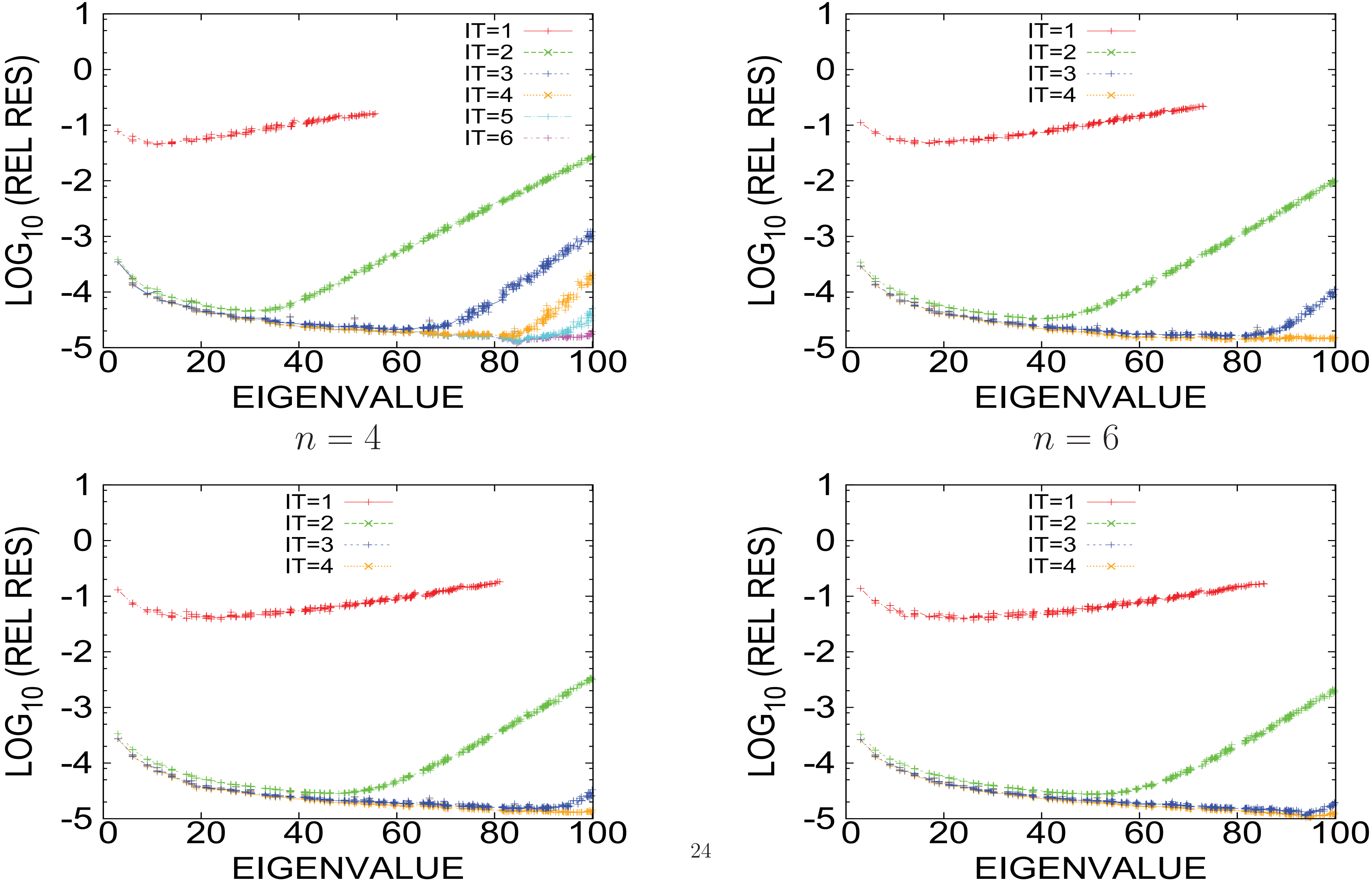
IT	# Eigenpairs	Max Rel Residual
1	286(286)	1.7E-01 (1.7E-01)
2	402(402)	2.1E-03 (2.4E-03)
3	402(402)	2.7E-04 (8.1E-06)
4	402(402)	2.6E-04 (2.4E-08)
5	402(402)	2.6E-04 (8.2E-11)
6	402(402)	2.6E-04 (1.2E-12)

(Data in parenthesis are from D-P calculations.)

(Ex-1, Lower-end Eigenpairs): Max of Relative Residuals



(Ex-1): Relative Residual (S-P calculation)



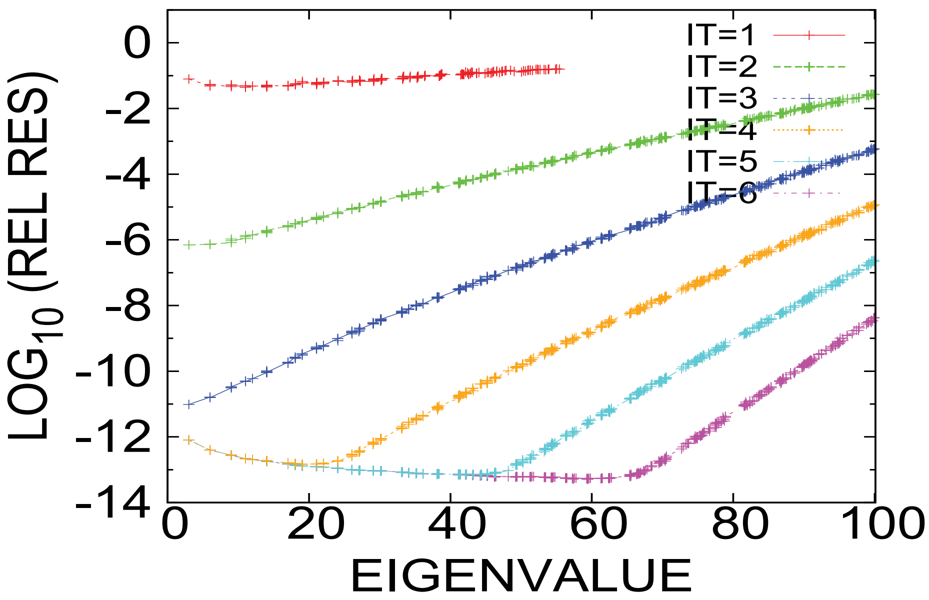
$n = 4$

$n = 6$

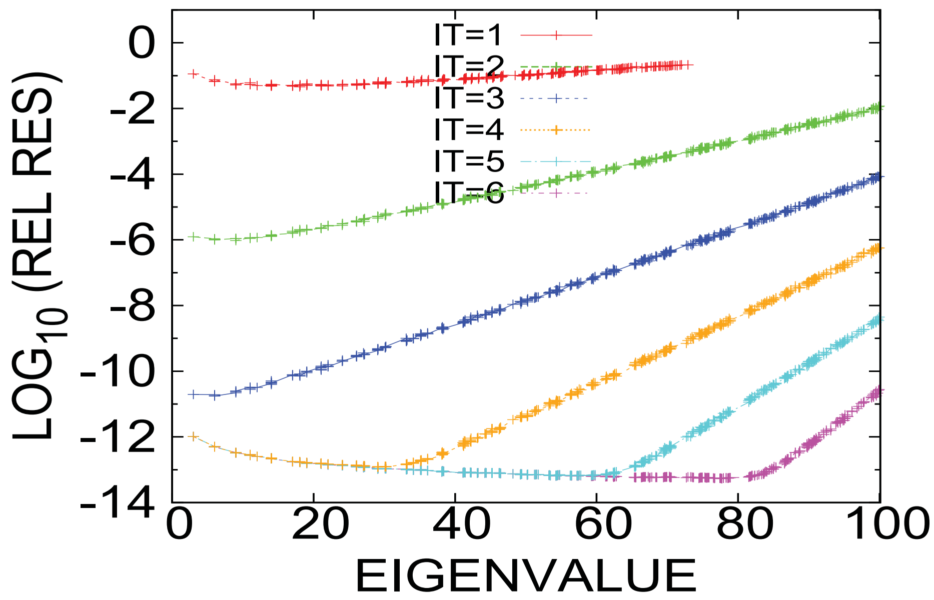
$n = 8$

$n = 10$

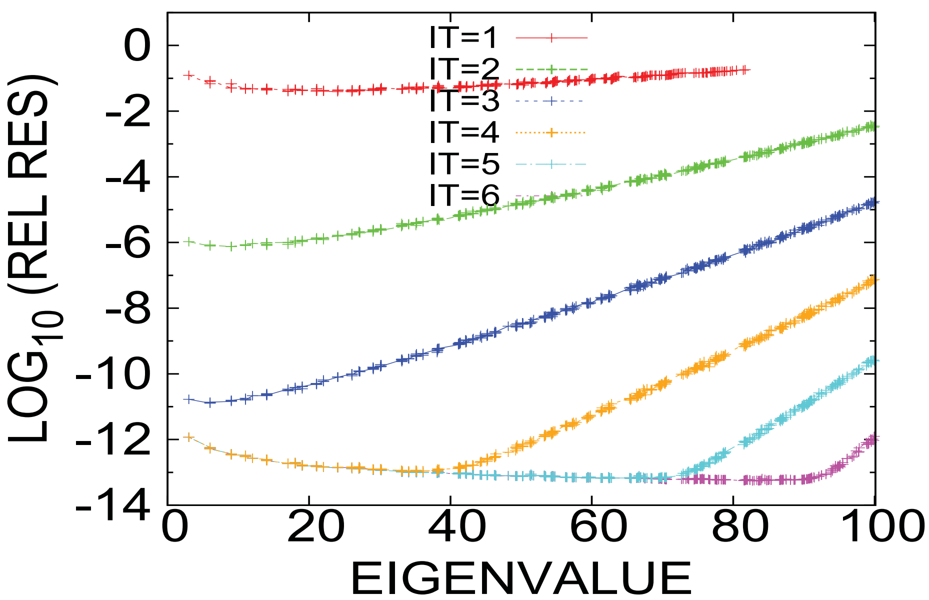
(Ex-1): Relative Residual (D-P calculation)



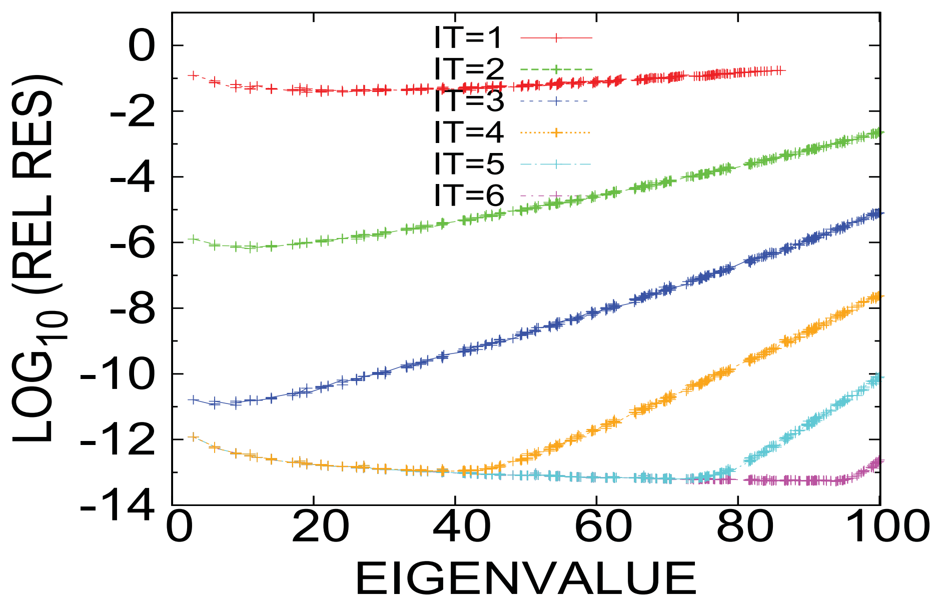
$n = 4$



$n = 6$

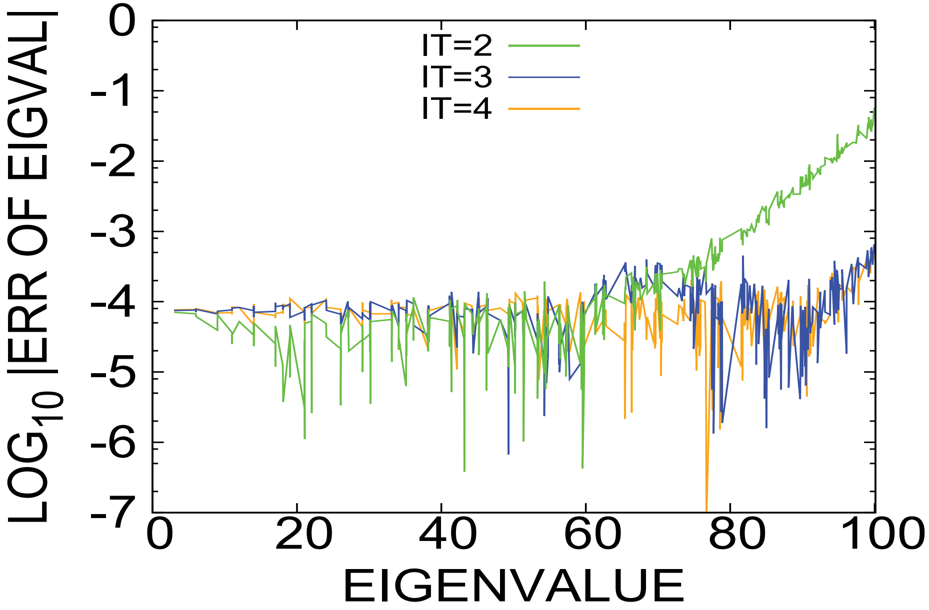


$n = 8$

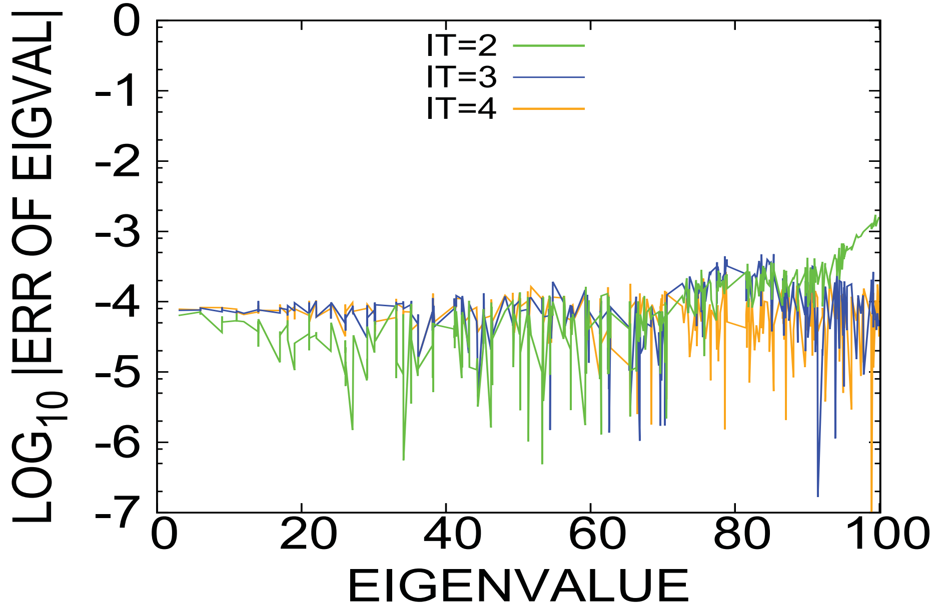


$n = 10$

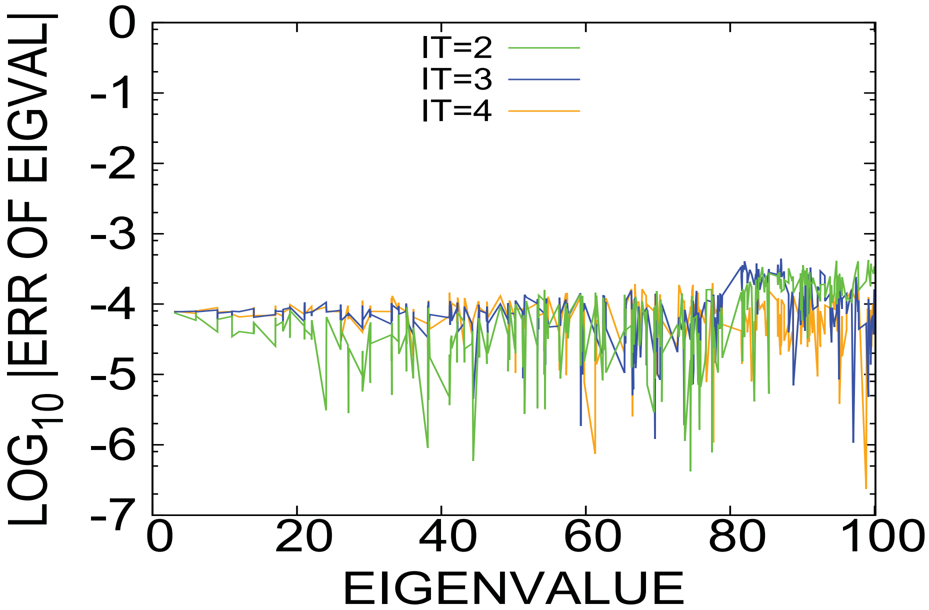
(Ex-1): Error of Eigenvalue (S-P calculation)



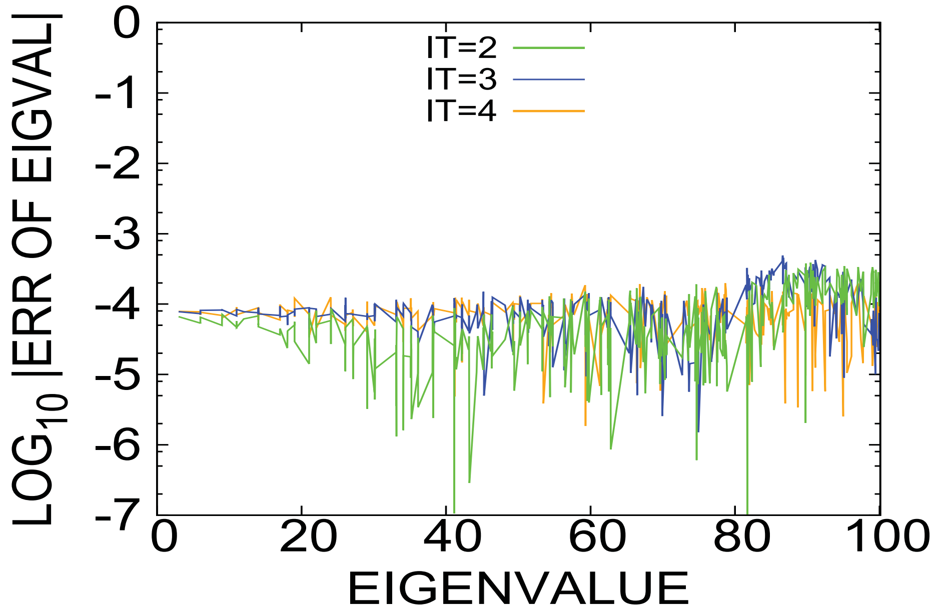
$n = 4$



$n = 6$

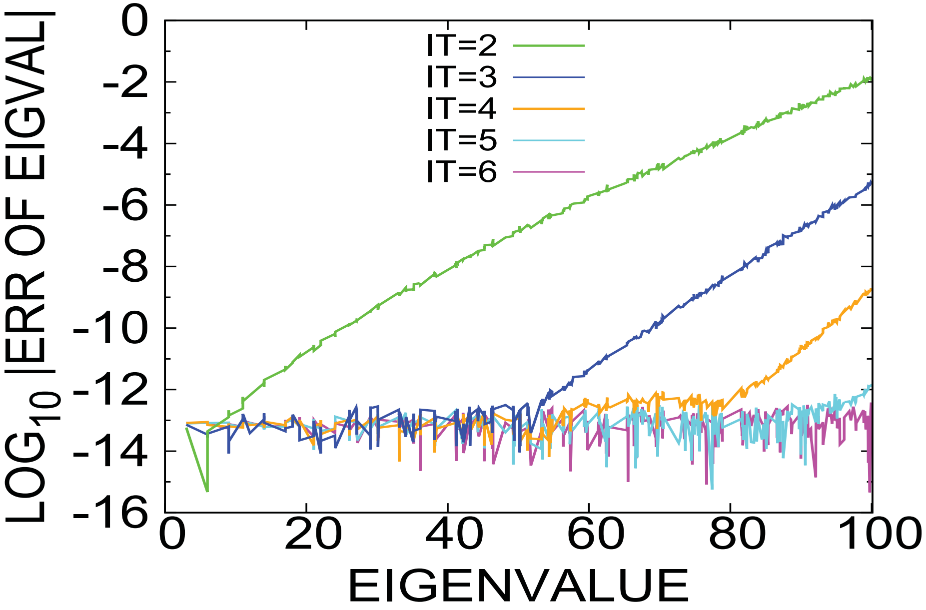


$n = 8$

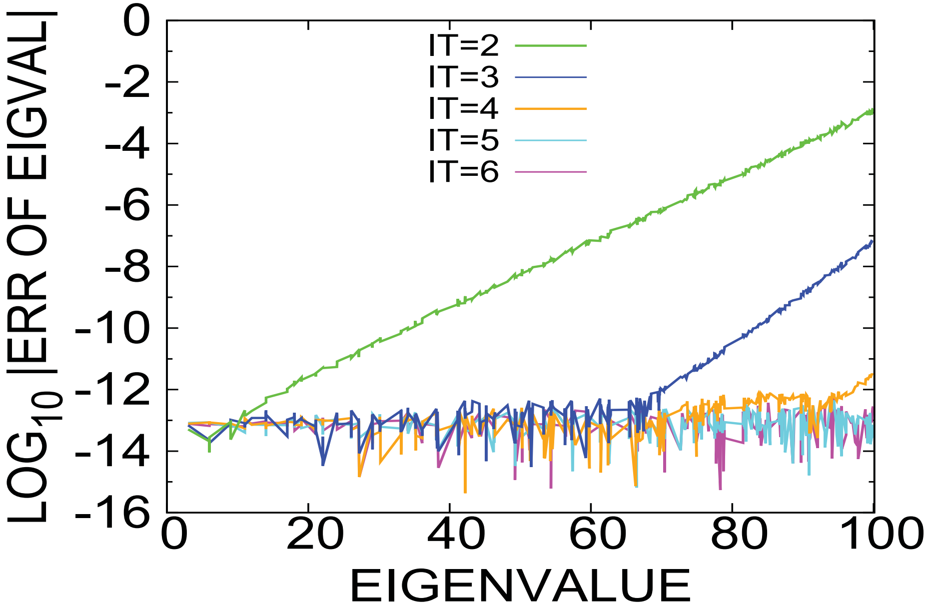


$n = 10$

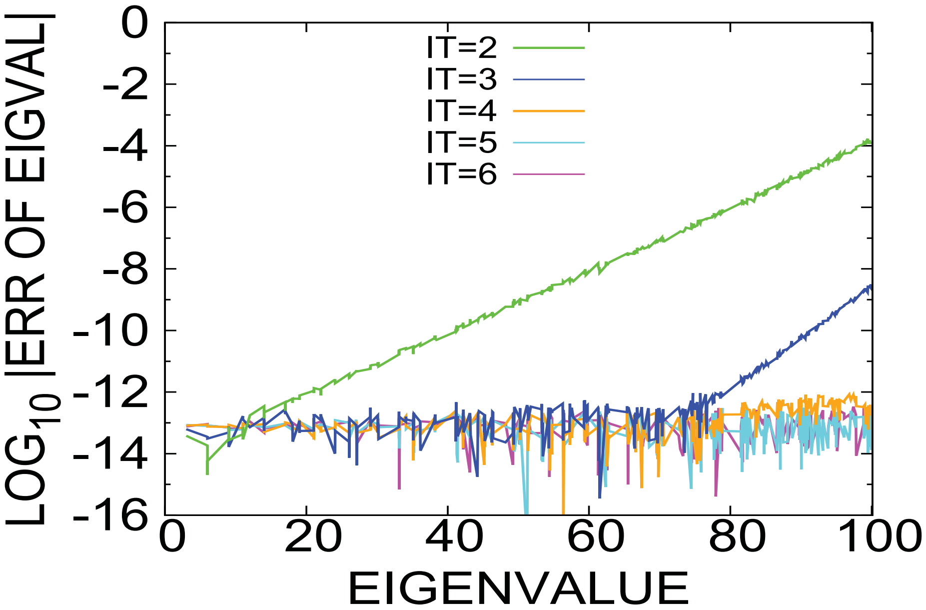
(Ex-1): Error of Eigenvalue (D-P calculation)



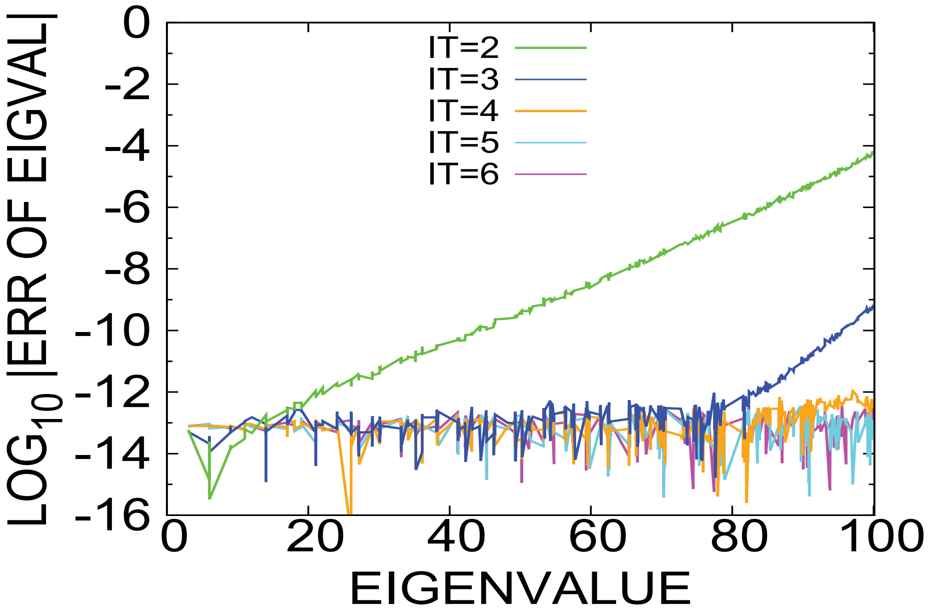
$n = 4$



$n = 6$



$n = 8$



$n = 10$

Elapsed Time in Seconds

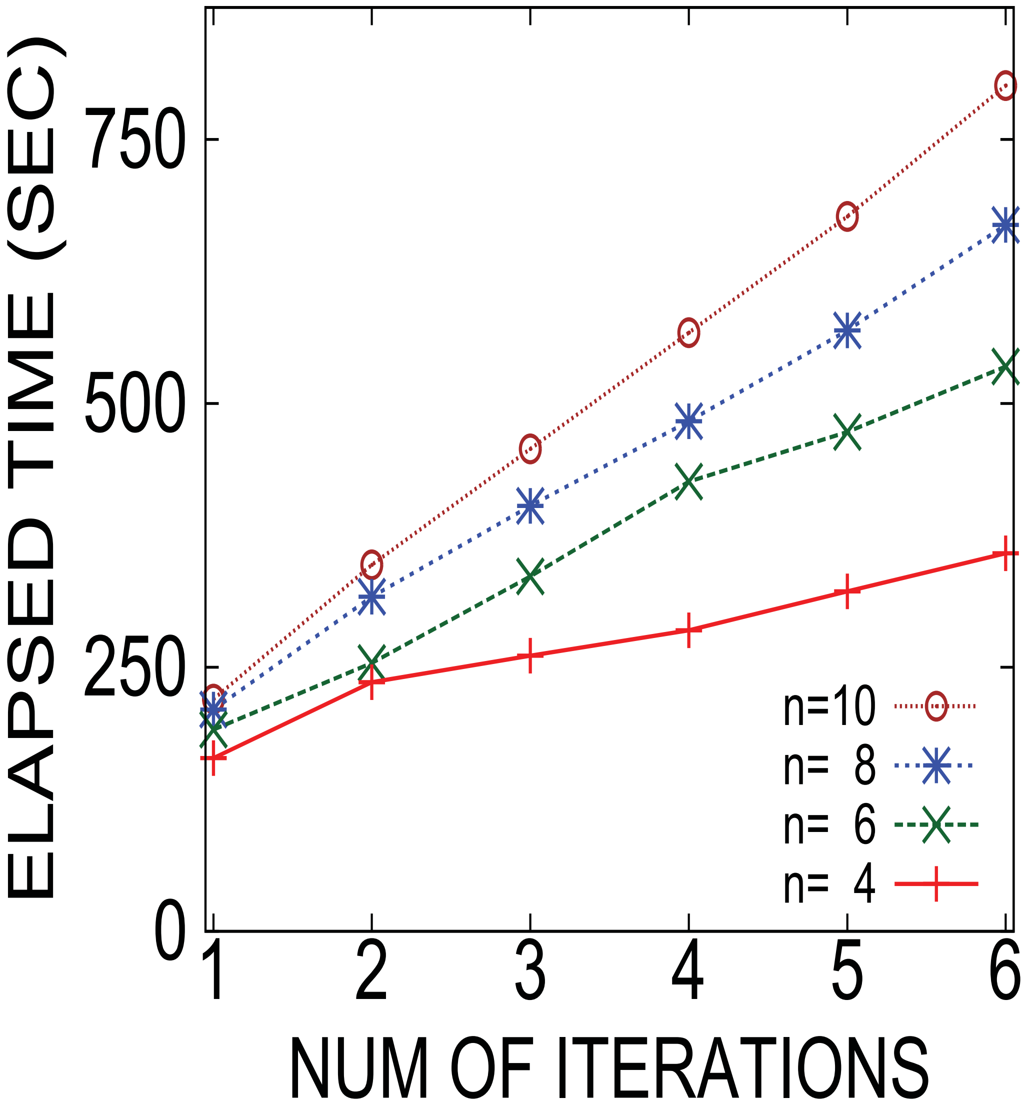
(Ex-1): For lower-end eigenpairs ($m = 800$ initial vectors)

IT	$n = 4$	$n = 6$	$n = 8$	$n = 10$
1	164(271)	191(314)	210(342)	220(403)
2	236(432)	254(510)	317(587)	347(678)
3	261(523)	336(650)	403(761)	457(885)
4	285(633)	426(792)	483(945)	567(1,114)
5	322(721)	473(918)	569(1,118)	677(1,330)
6	358(818)	535(1,070)	669(1,306)	801(1,551)

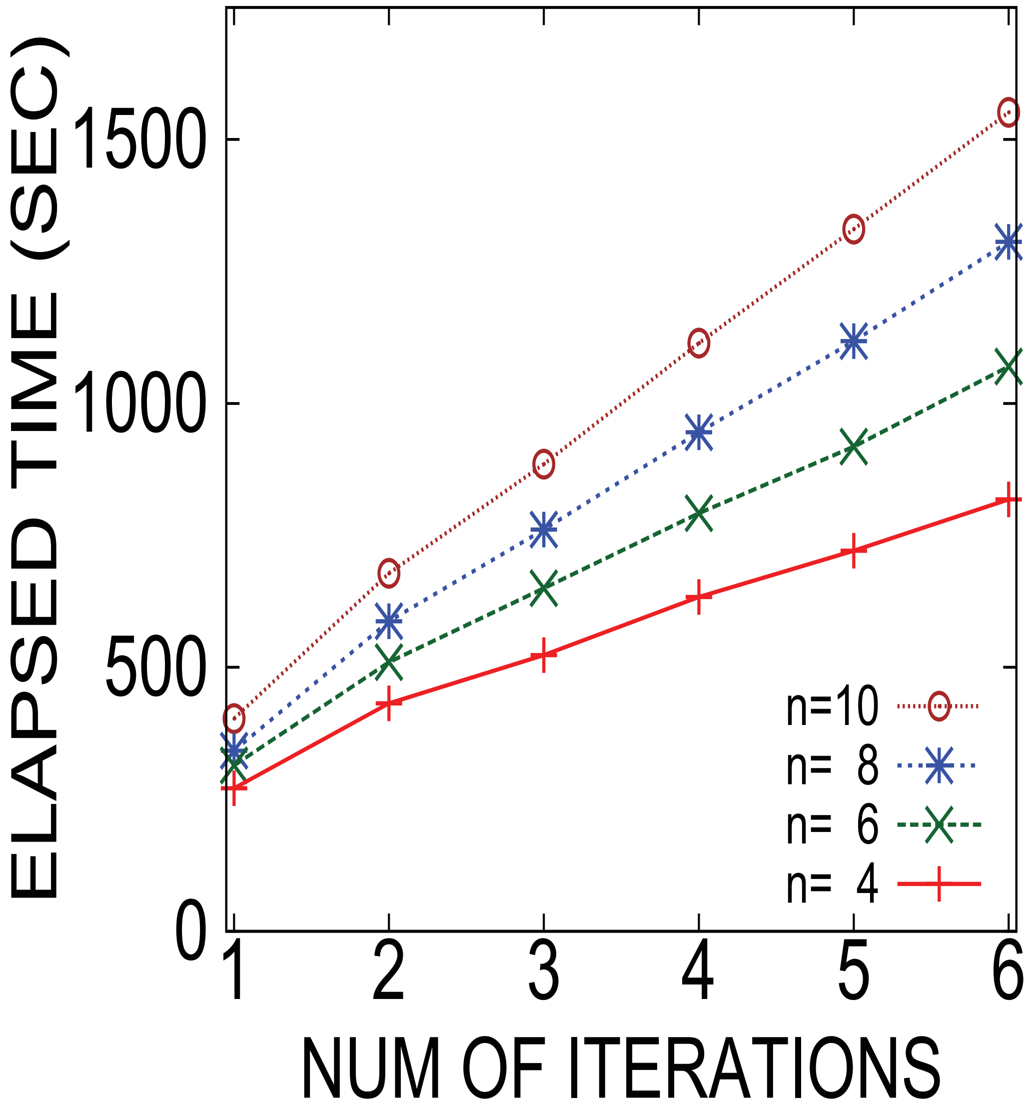
(Data in parenthesis are from D-P calculations.)

(Ex-1, Lower-end Eigenpairs): Elapsed Time in Seconds

S-P calculation



D-P calculation



Ex-2 : INTERIOR EIGENPAIRS

(Ex-2): Solution of Interior Eigenpairs

- **In the interior interval** $[\,a,\,b\,] = [\,100,\,200\,]$**,** **there are** 801 **eigenpairs to be solved.**

- **The union of the pass-band and transition-bands** $[\,a',\,b'\,] = [\,75,\,225\,]$ **contains** $1,192$ **eigenvalues.**

- **The number of initial vectors used :** $m = 1,300$**.** **(More than** $1,192$ **and would be sufficient.)**

- **The results of experiment are shown.**

(Ex-2): Num of Approx Eigenpairs and Max Rel Residuals

($\mu = 1.5$, $g_{\mathtt{s}} = \mathtt{1E\text{-}5}$, $m = 1,300$, the correct num of pairs is 801).

$n = 4$

IT	# Eigenpairs	Max Rel Residual
1	700(703)	3.1E-01 (2.9E-01)
2	801(801)	2.3E-03 (2.5E-03)
3	801(801)	3.6E-05 (7.5E-06)
4	801(801)	2.2E-05 (2.1E-08)

$n = 6$

IT	# Eigenpairs	Max Rel Residual
1	800(799)	3.3E-01 (3.4E-01)
2	801(801)	2.2E-04 (2.2E-04)
3	801(801)	2.3E-05 (1.8E-07)
4	801(801)	2.3E-05 (1.5E-10)

$n = 8$

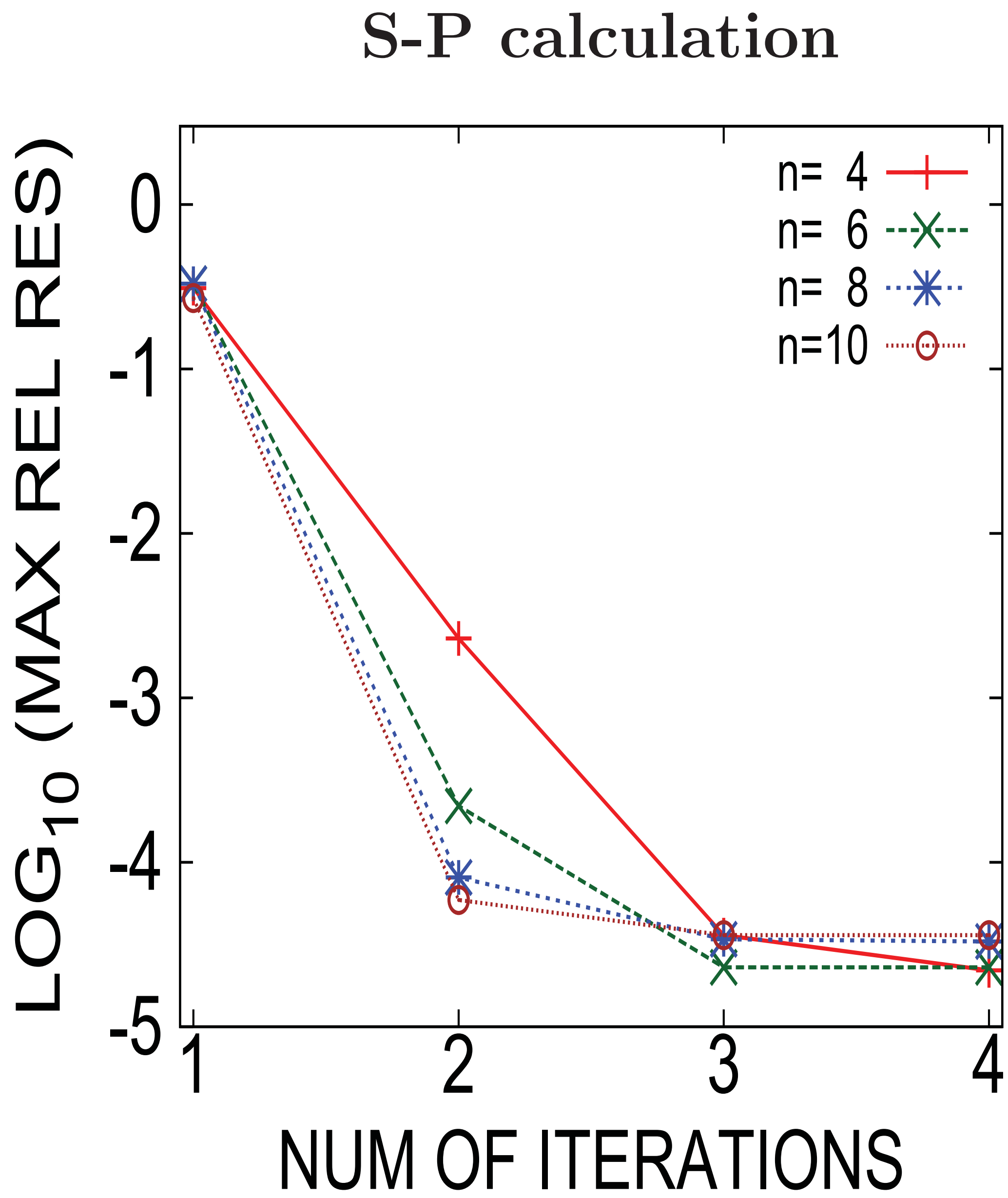
IT	# Eigenpairs	Max Rel Residual
1	824(787)	3.3E-01 (2.8E-01)
2	801(801)	8.1E-05 (6.8E-05)
3	801(801)	3.4E-05 (3.3E-08)
4	801(801)	3.3E-05 (1.6E-11)

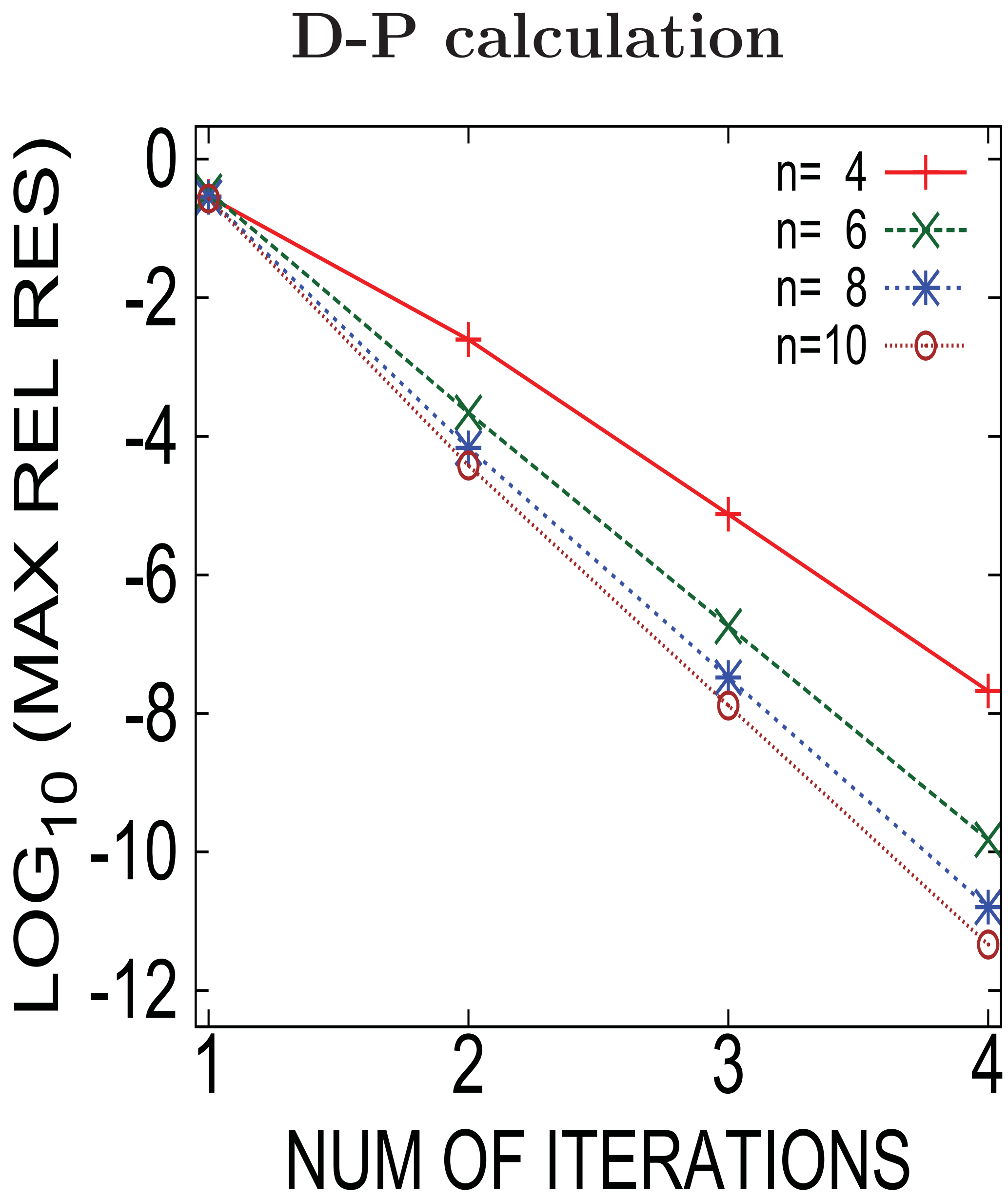
$n = 10$

IT	# Eigenpairs	Max Rel Residual
1	828(829)	2.7E-01 (2.7E-01)
2	801(801)	5.9E-05 (3.8E-05)
3	801(801)	3.6E-05 (1.3E-08)
4	801(801)	3.6E-05 (4.6E-12)

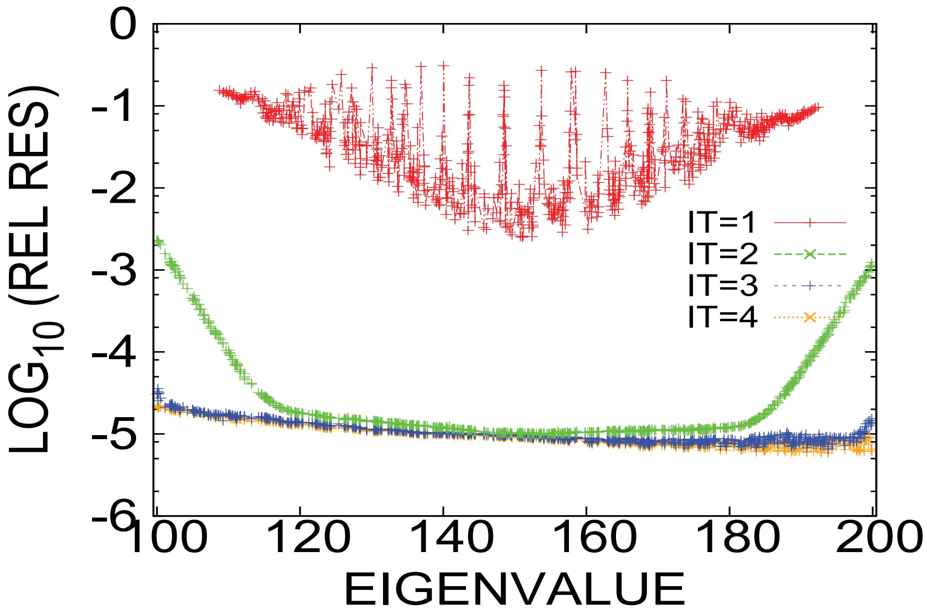
(Data in parenthesis are from D-P calculations.)

(Ex-2, Interior Eigenpairs): Max of Relative Residuals

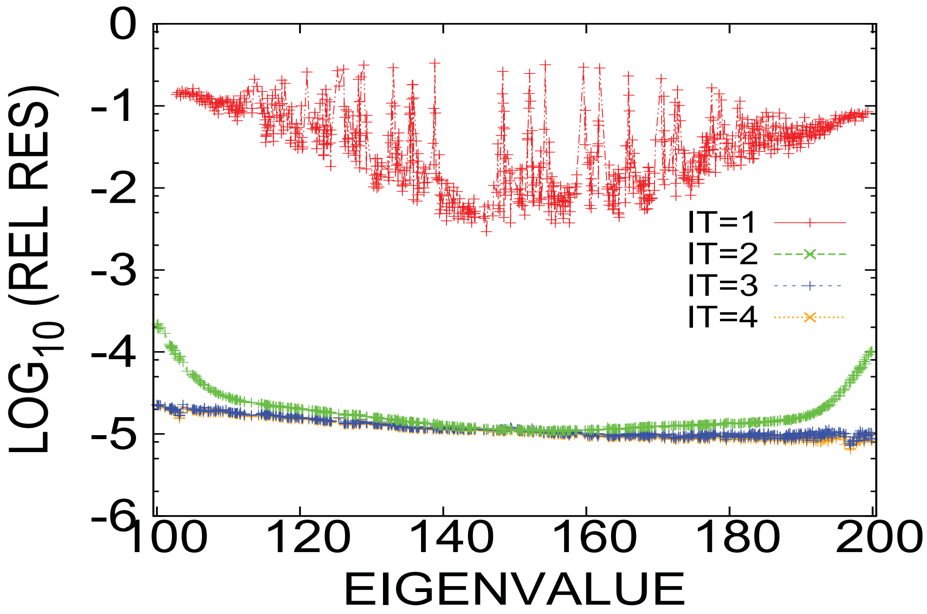




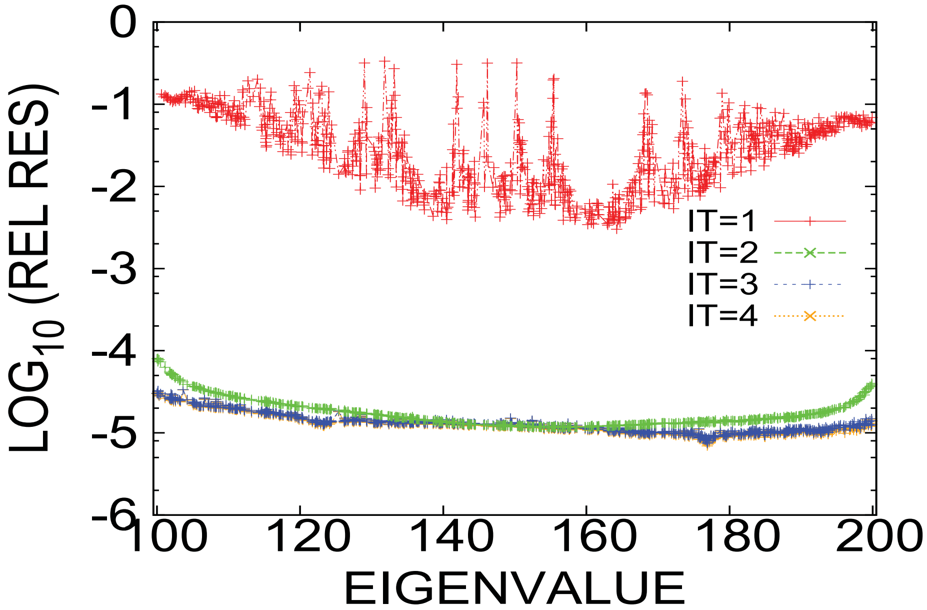
(Ex-2): Relative Residual (S-P calculation)



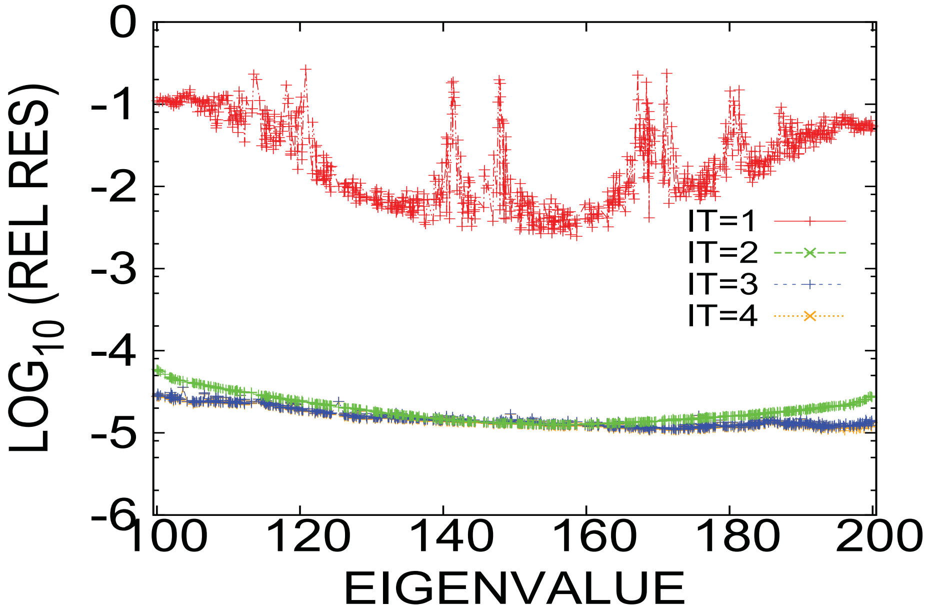
$n = 4$



$n = 6$

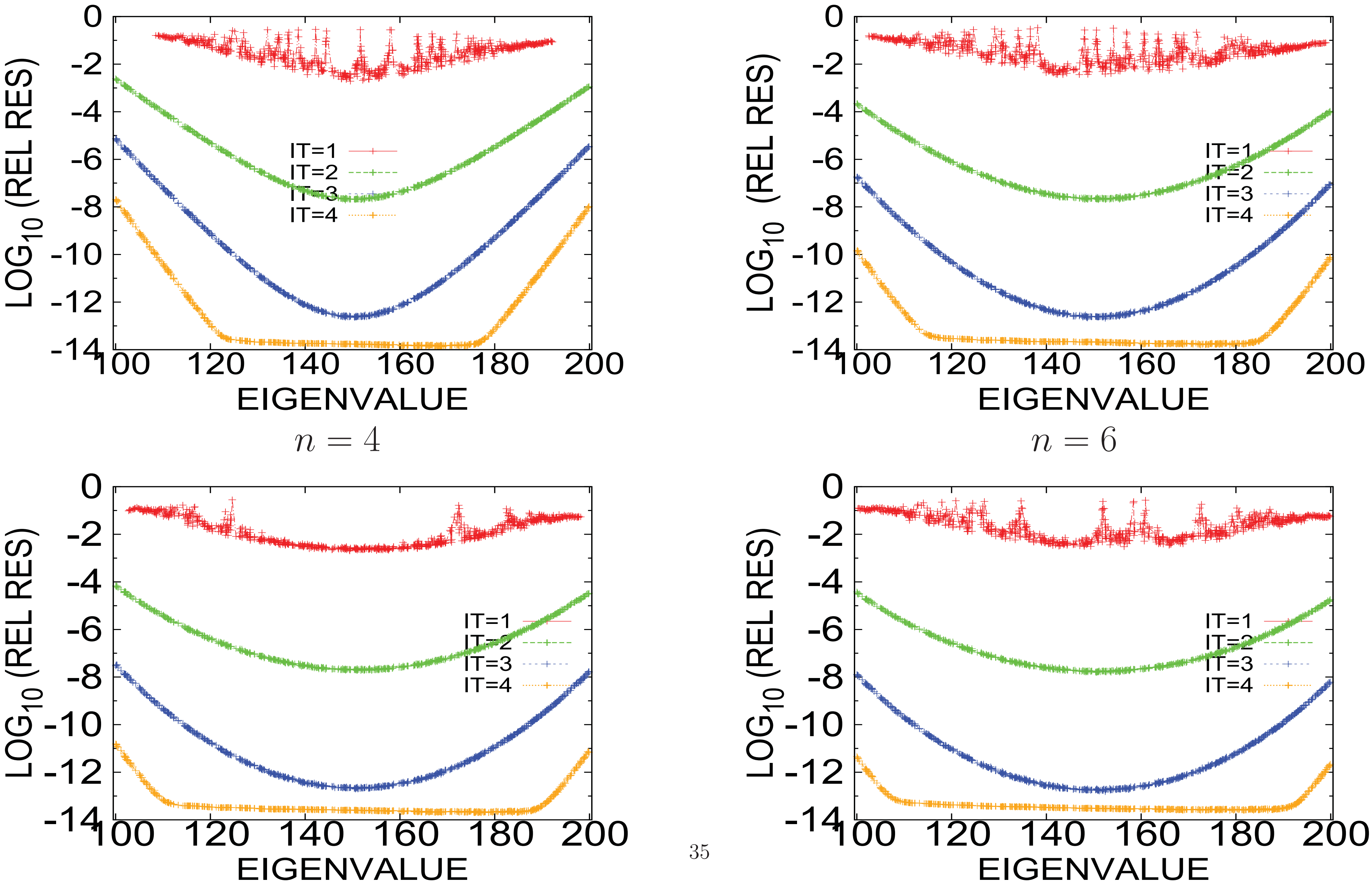


$n = 8$



$n = 10$

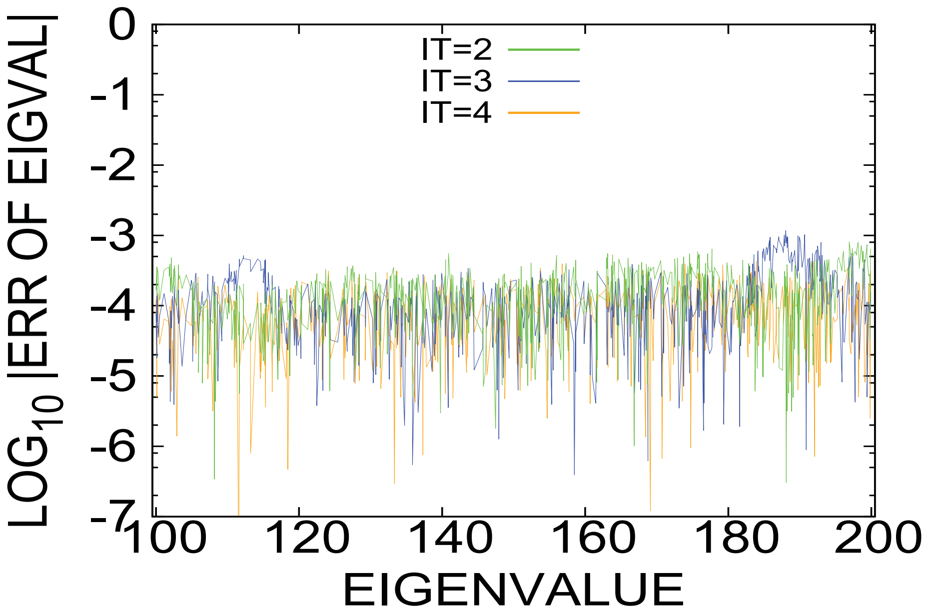
(Ex-2): Relative Residual (D-P calculation)



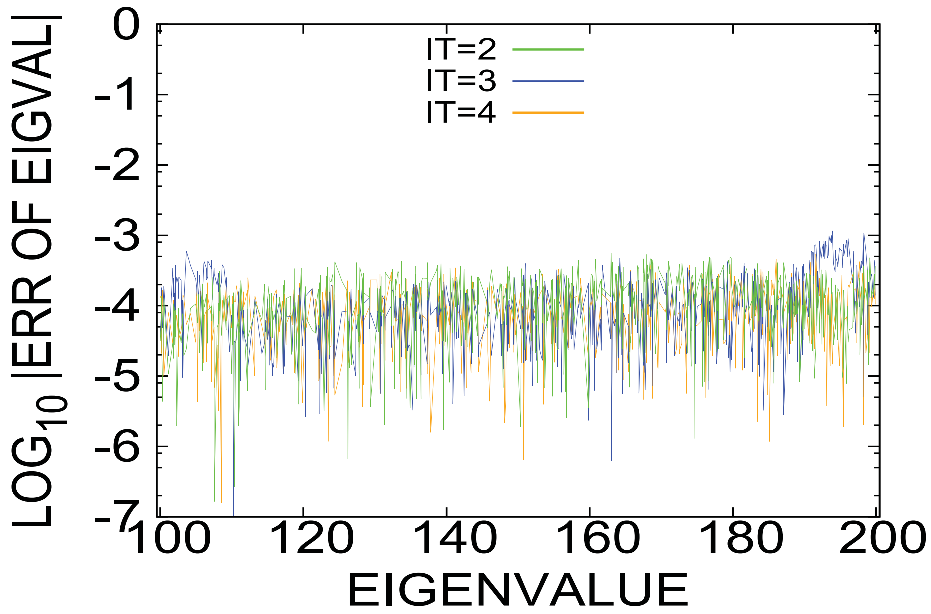
$n = 4$ $n = 6$

$n = 8$ $n = 10$

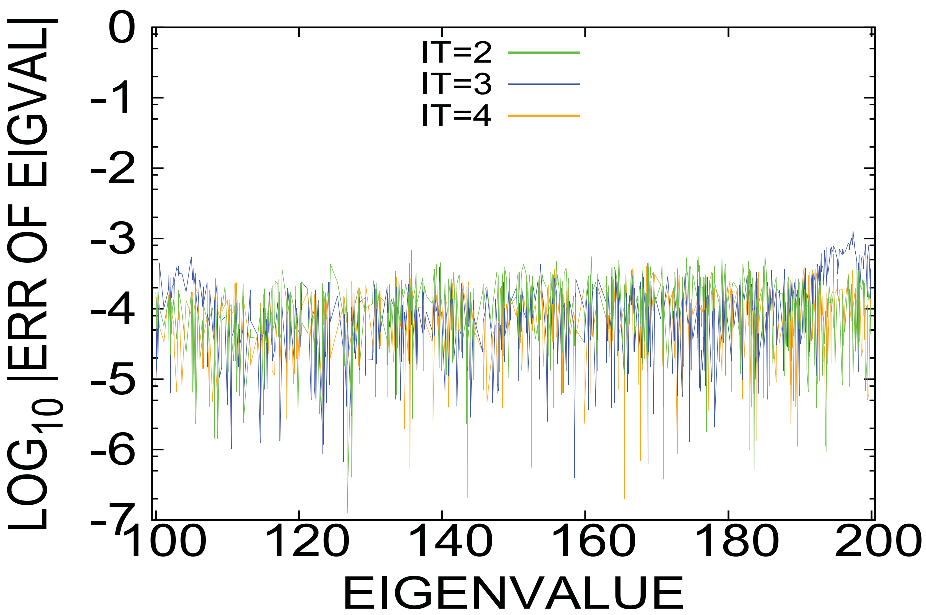
(Ex-2): Error of Eigenvalue (S-P calculation)



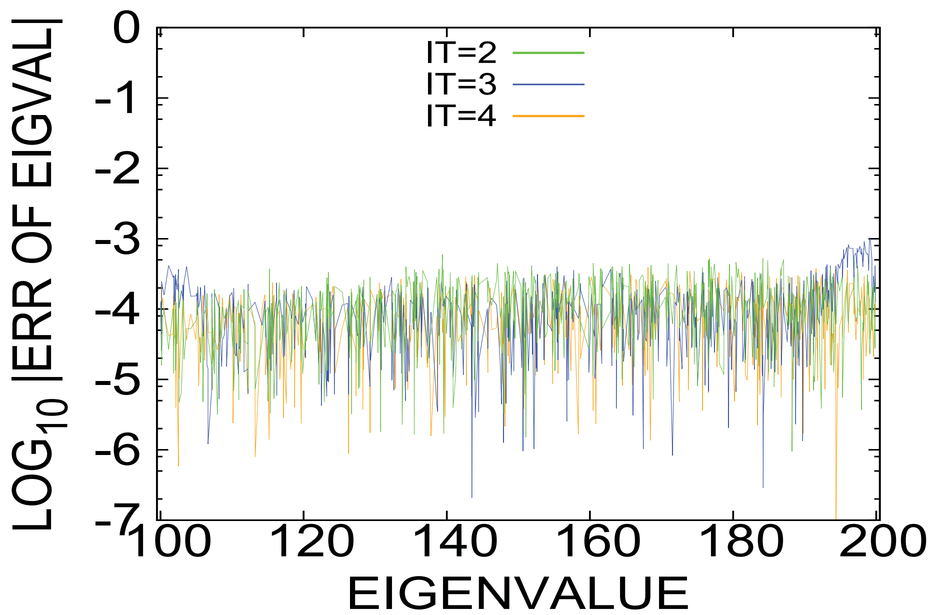
$n = 4$



$n = 6$

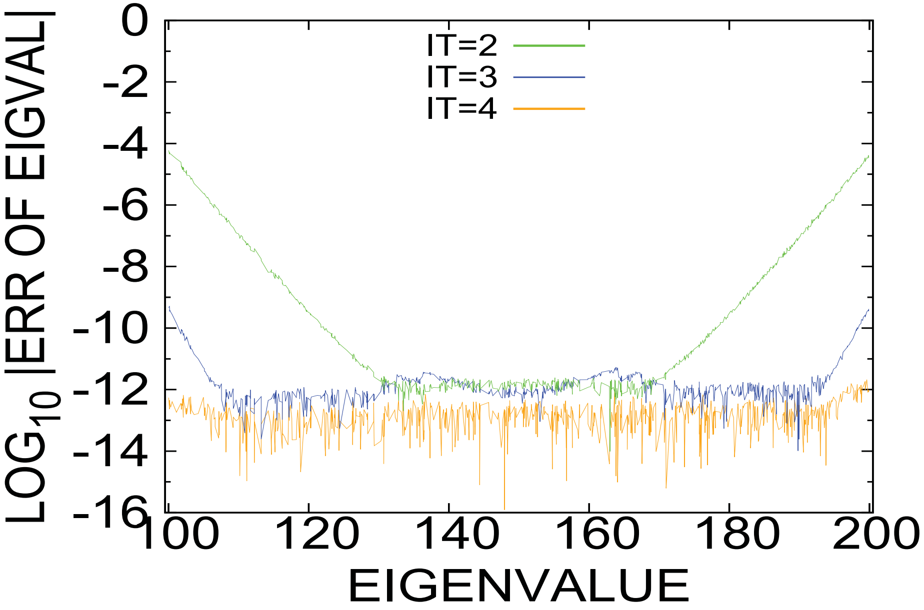


$n = 8$

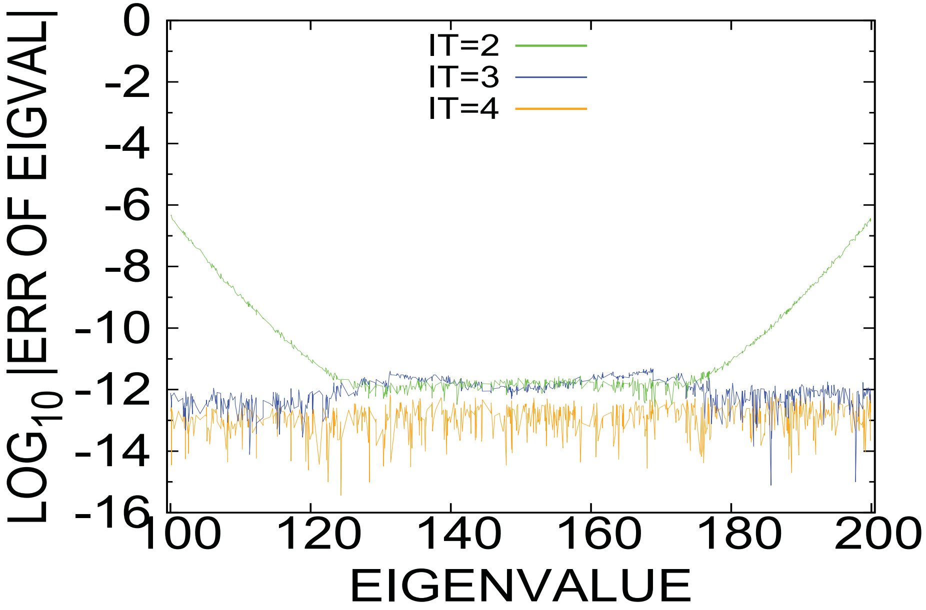


$n = 10$

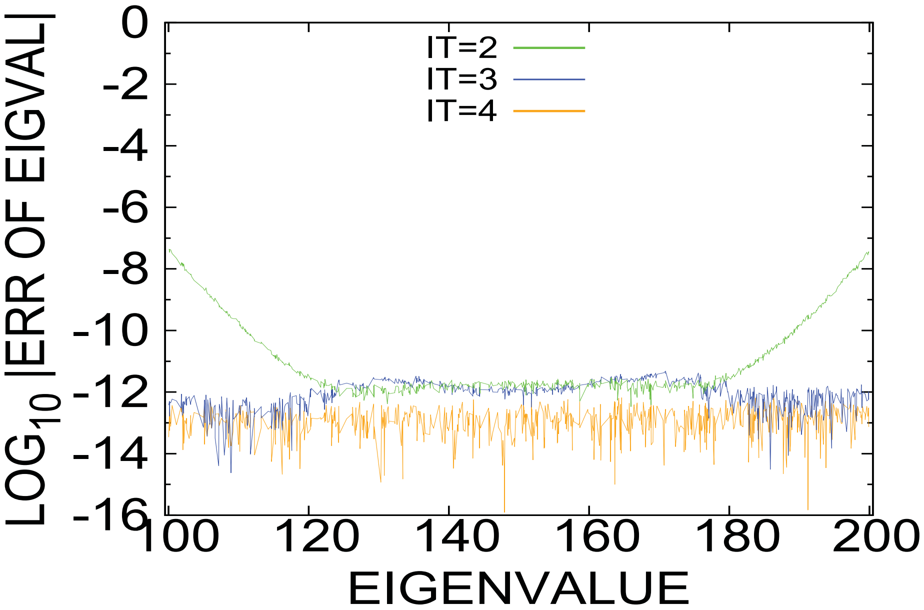
(Ex-2): Error of Eigenvalue (D-P calculation)



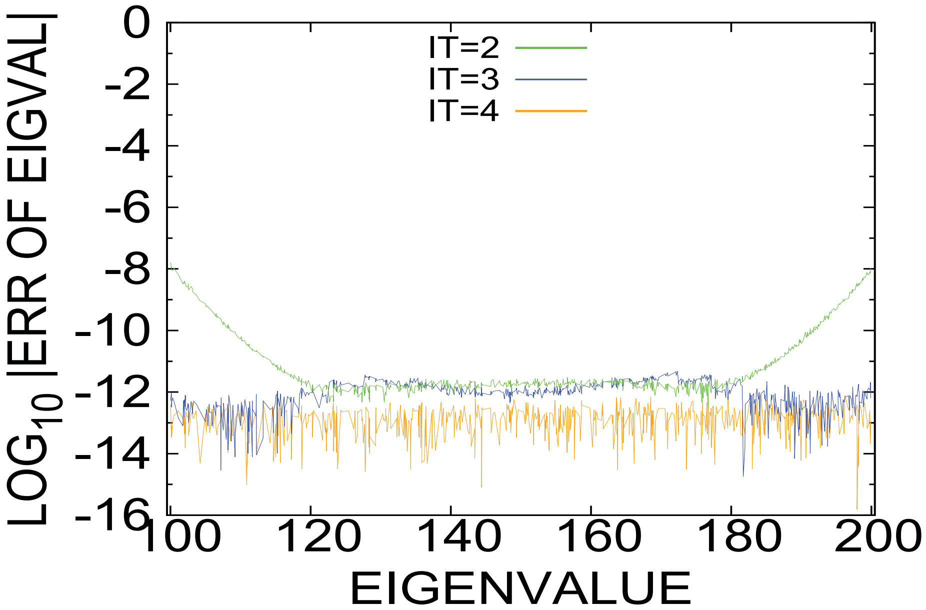
$n = 4$



$n = 6$



$n = 8$



$n = 10$

Elapsed Time in Seconds

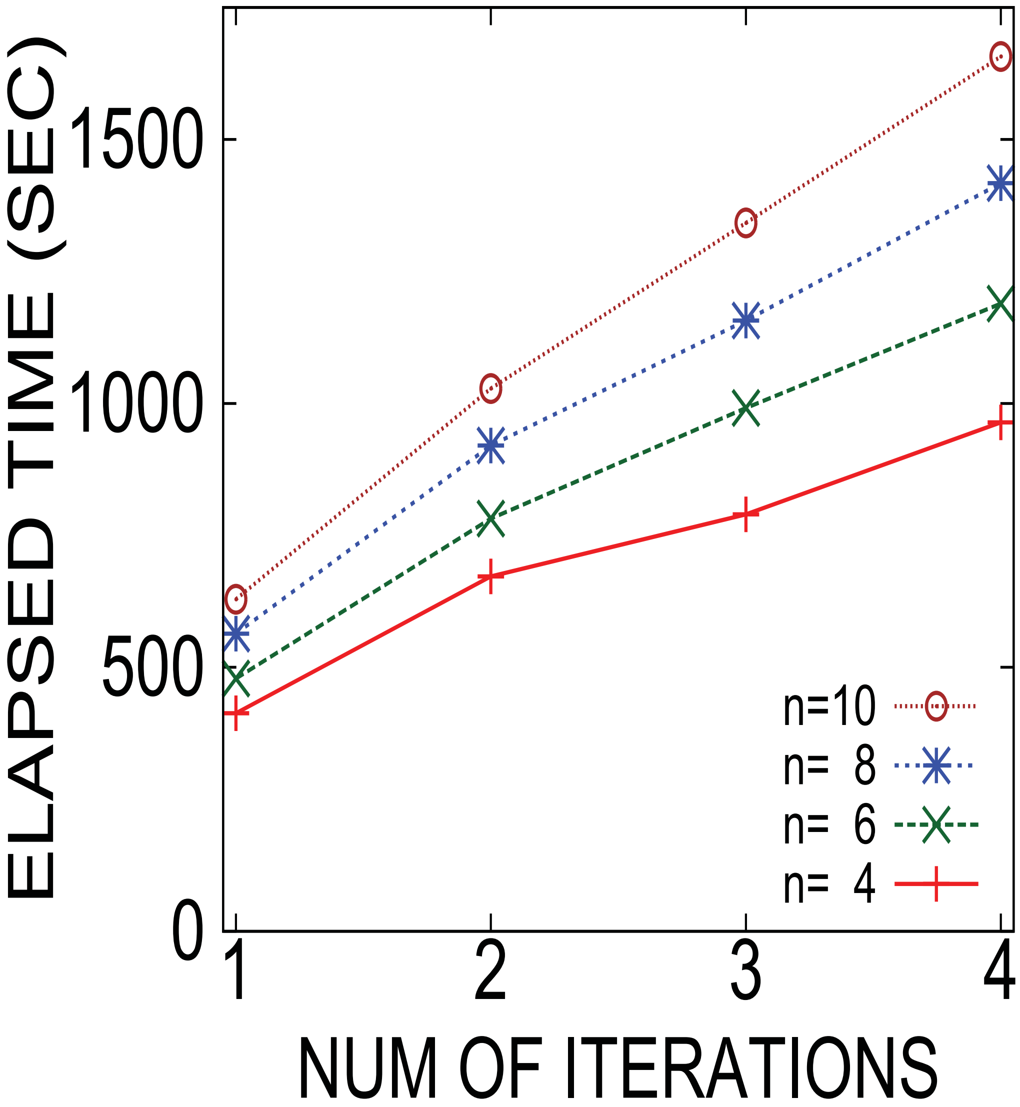
(Ex-2): For interior eigenpairs ($m = 1,300$ initial vectors)

IT	$n=4$	$n=6$	$n=8$	$n=10$
1	413(690)	479(837)	564(969)	629(1,121)
2	672(1,132)	782(1,390)	920(1,657)	1,028(1,931)
3	790(1,435)	991(1,841)	1,157(2,234)	1,342(2,631)
4	964(1,741)	1,189(2,275)	1,417(2,803)	1,657(3,333)

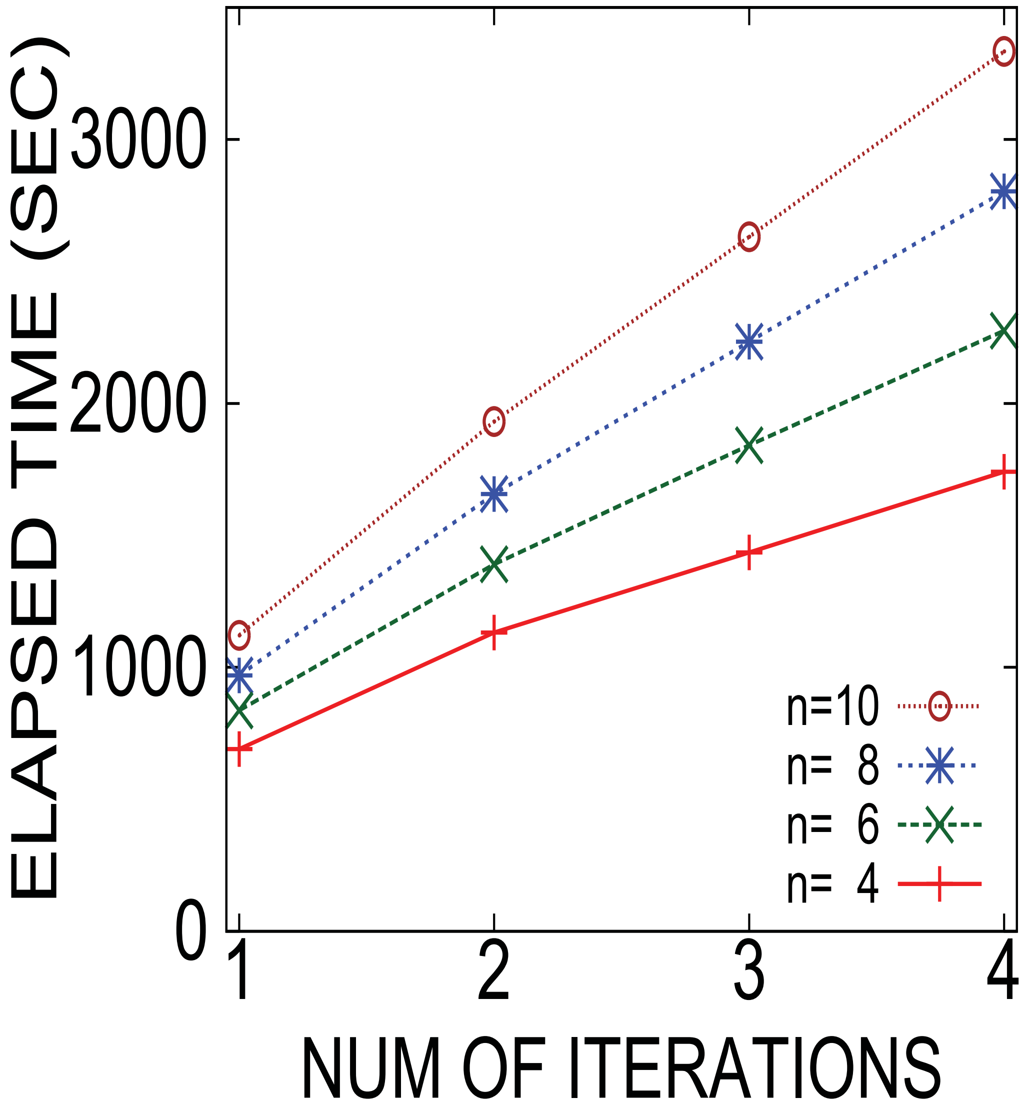
(Data in parenthesis are from D-P calculations.)

(Ex-2, Interior Eigenpairs): Elapsed Time in Seconds

S-P calculation



D-P calculation



CONCLUSION

CONCLUSION

- We made experiments to solve a GEVP by using a filter. The GEVP tested was derived from a FEM discretization of the Laplace eigenvalue problem on the cube.
- To minimize resource requirements especially storage, we used filters composed of only a single resolvent. However, such filters have poor transfer properties.
- The present iterative approach to improve eigenpairs worked well to overcome the poor properties of the filters, even when the calculation was performed in S-P.
- On a system of intel Xeon Phi 7250 (KNL), we observed that both storage requirement and elapsed time of S-P calculation were about half of those of D-P calculation.

APPENDIX

TEST PROBLEM OF

HIGHLY DEGENERATE EIGENVALUES

Test Problem with Highly Degenerated Eigenvalues

- **The FEM partitioning :** $(N_1,\ N_2,\ N_3) = (60,\ 60,\ 60)$
  (This EVP has many 6-fold degenerated eigenvalues.)
- **Matrix** A **and** B **:**
  Size $N = 216,000$**, Lower-bandwidth** $w_L = 3,661$**.**
- **Solve eigenpairs whose eigenvalues are in the interval : lower-end** $[0, 100]$ **(Ex-1b), and interior** $[100, 200]$ **(Ex-2b).**
- **Designes of the filters are the same as Ex-1 and Ex-2.**
  $\mu = 1.5$**,** $g_{\mathrm{S}} = \texttt{1E-5}$**, and the degree** n **is 4, 6, 8 and 10.**
- **The correct number of eigenpairs :**
  404 (Ex-1b), and 798 (Ex-2b).
- **The number of initial random vectors :**
  $m = 800$ **(Ex-1b), and** $m = 1,300$ **(Ex-2b).**

Ex-1b : LOWER-END EIGENPAIRS

(Ex-1b): Num of Approx Eigenpairs and Max Rel Residuals

($\mu = 1.5$, $g_{\mathtt{s}} = \mathtt{1E\text{-}5}$, $m = 800$, the correct num eigenpairs is 404).

$n = 4$

IT	# Eigenpairs	Max Rel Residual
1	<u>139</u>(<u>140</u>)	1.6E-01 (1.6E-01)
2	404(404)	2.9E-02 (2.9E-02)
3	404(404)	1.6E-03 (6.4E-04)
4	404(404)	3.3E-04 (1.3E-05)
5	404(404)	3.3E-04 (2.5E-07)
6	404(404)	3.3E-04 (4.5E-09)

$n = 6$

IT	# Eigenpairs	Max Rel Residual
1	<u>219</u>(<u>219</u>)	2.2E-01 (2.2E-01)
2	404(404)	1.1E-02 (1.2E-02)
3	404(404)	2.8E-04 (9.8E-05)
4	404(404)	2.8E-04 (6.7E-07)
5	404(404)	2.8E-04 (4.5E-09)
6	404(404)	2.8E-04 (2.6E-11)

$n = 8$

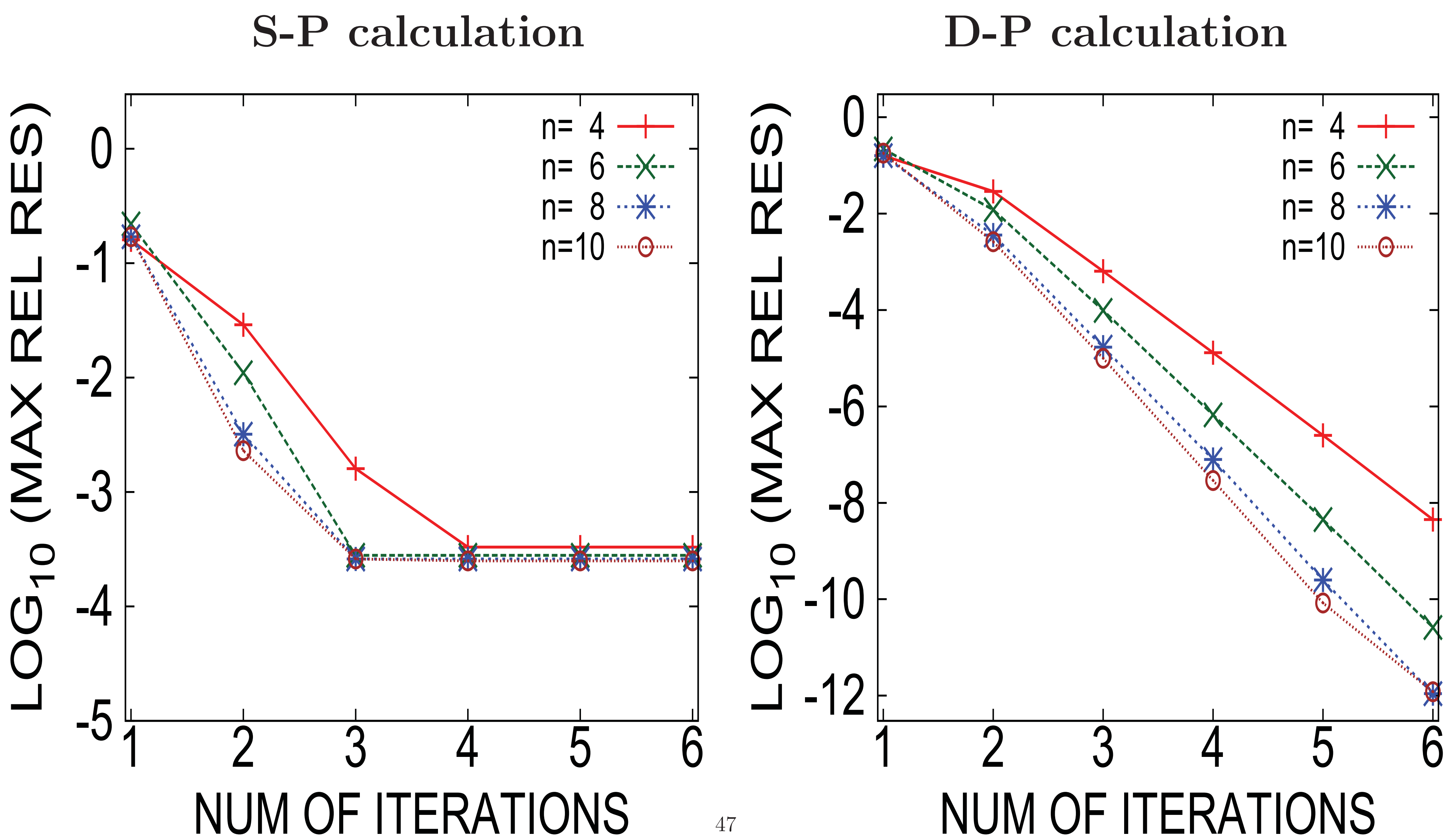
IT	# Eigenpairs	Max Rel Residual
1	<u>264</u>(<u>264</u>)	1.7E-01 (1.6E-01)
2	404(404)	3.2E-03 (3.6E-03)
3	404(404)	2.6E-04 (1.7E-05)
4	404(404)	2.6E-04 (7.9E-08)
5	404(404)	2.6E-04 (2.5E-10)
6	404(404)	2.6E-04 (1.1E-12)

$n = 10$

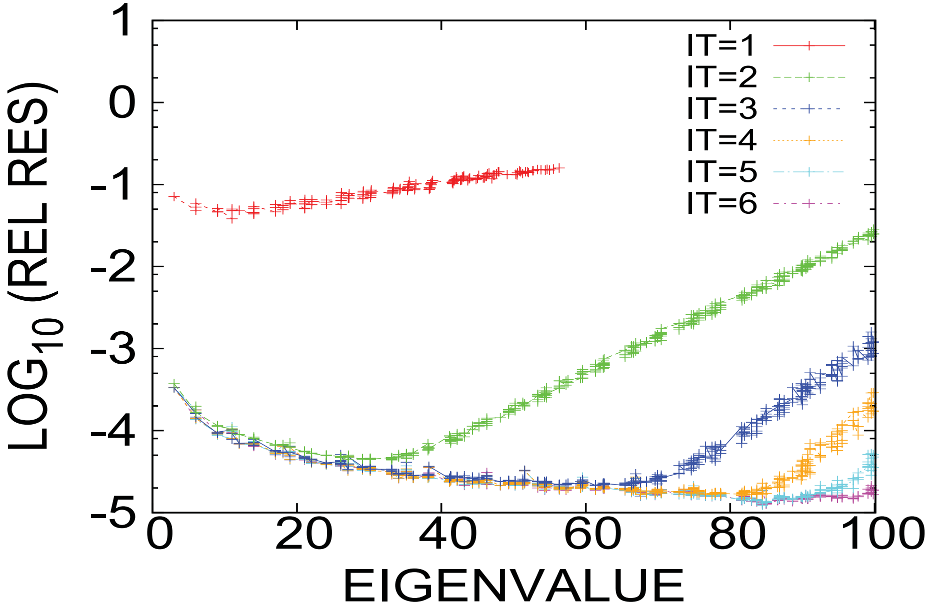
IT	# Eigenpairs	Max Rel Residual
1	<u>286</u>(<u>285</u>)	1.7E-01 (1.8E-01)
2	404(404)	2.3E-03 (2.6E-03)
3	404(404)	2.6E-04 (1.0E-05)
4	404(404)	2.5E-04 (2.9E-08)
5	404(404)	2.5E-04 (8.4E-11)
6	404(404)	2.5E-04 (1.2E-12)

(Data in parenthesis are from D-P calculations.)

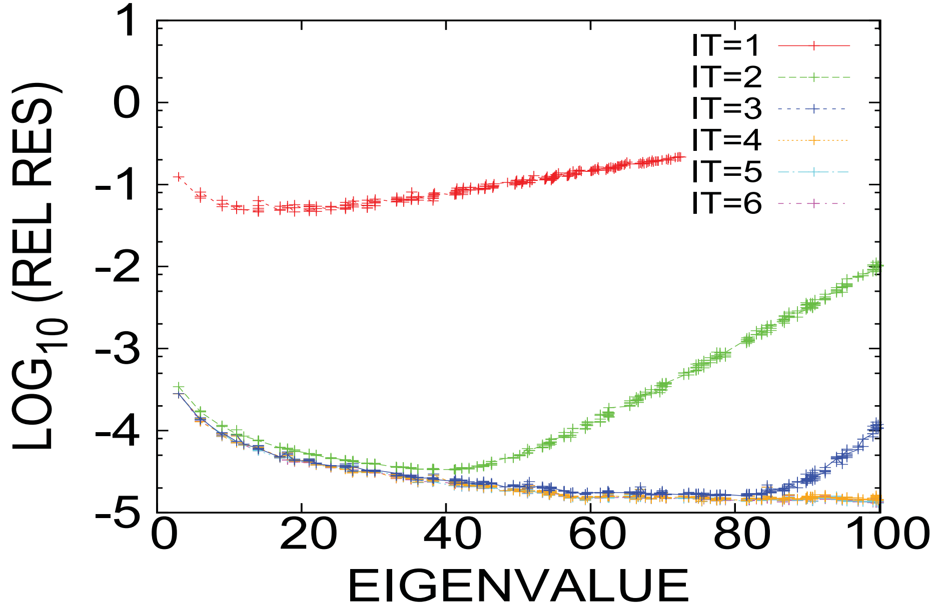
(Ex-1b, Lower-end Eigenpairs): Max of Relative Residuals



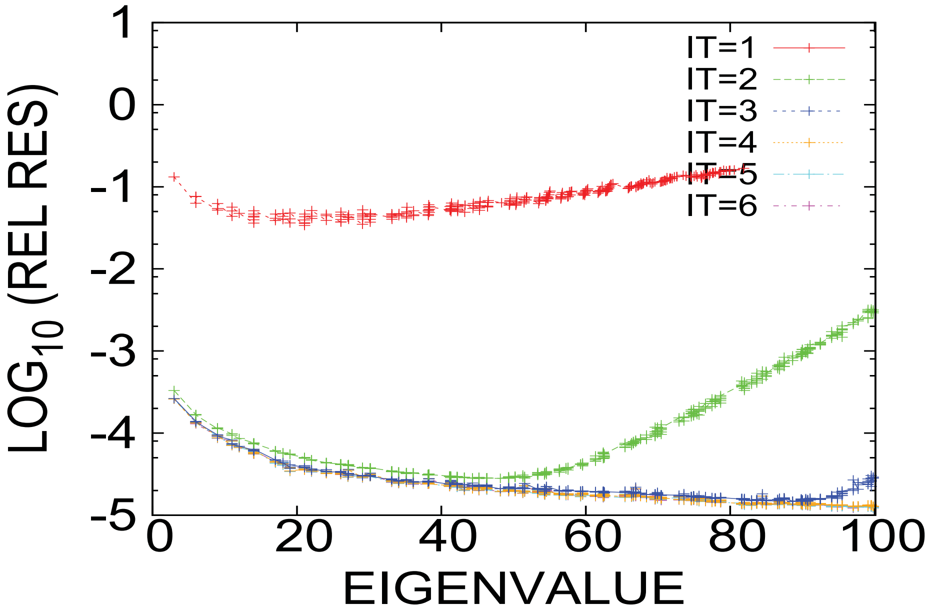
(Ex-1b): Relative Residual (S-P calculation)



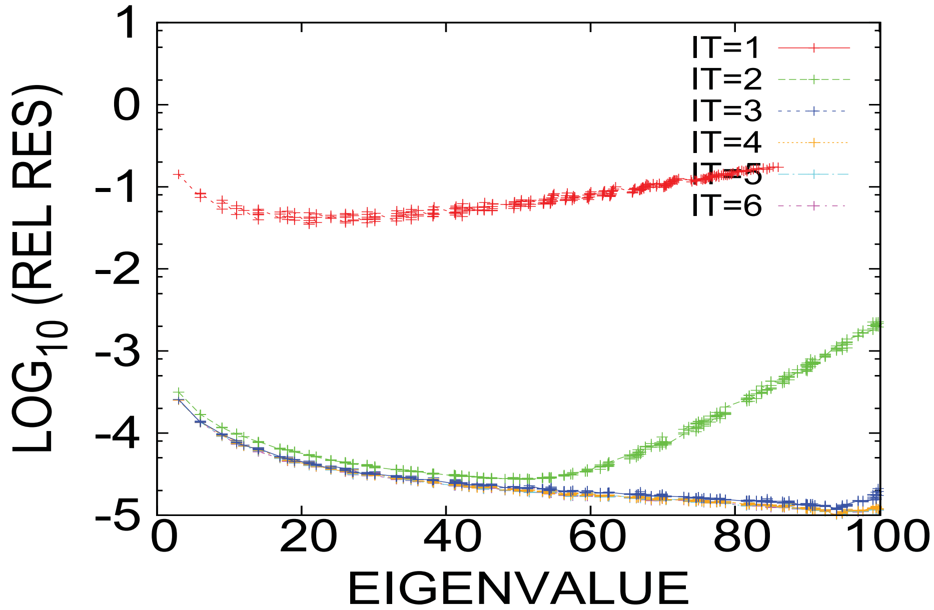
$n = 4$



$n = 6$

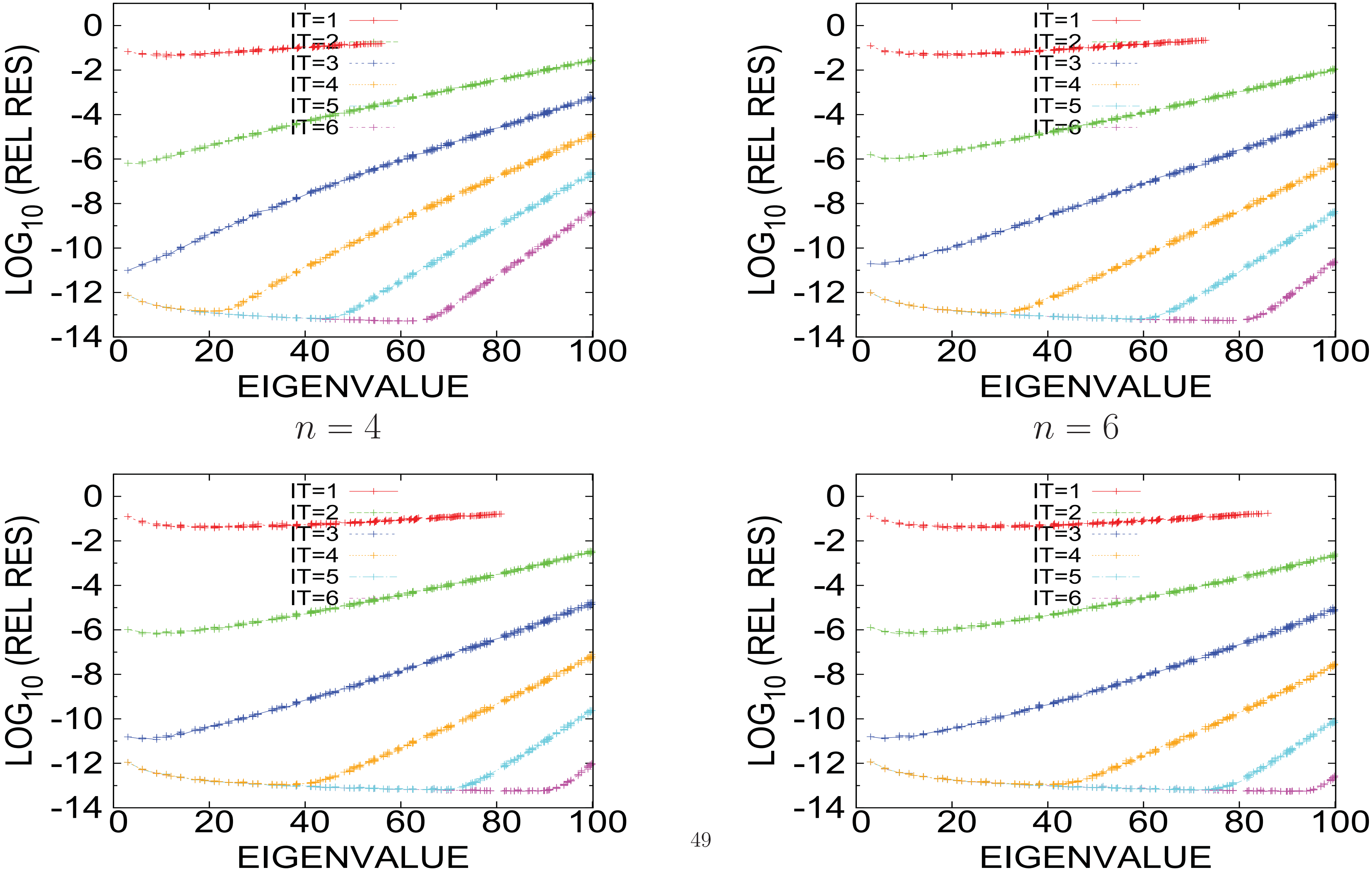


$n = 8$



$n = 10$

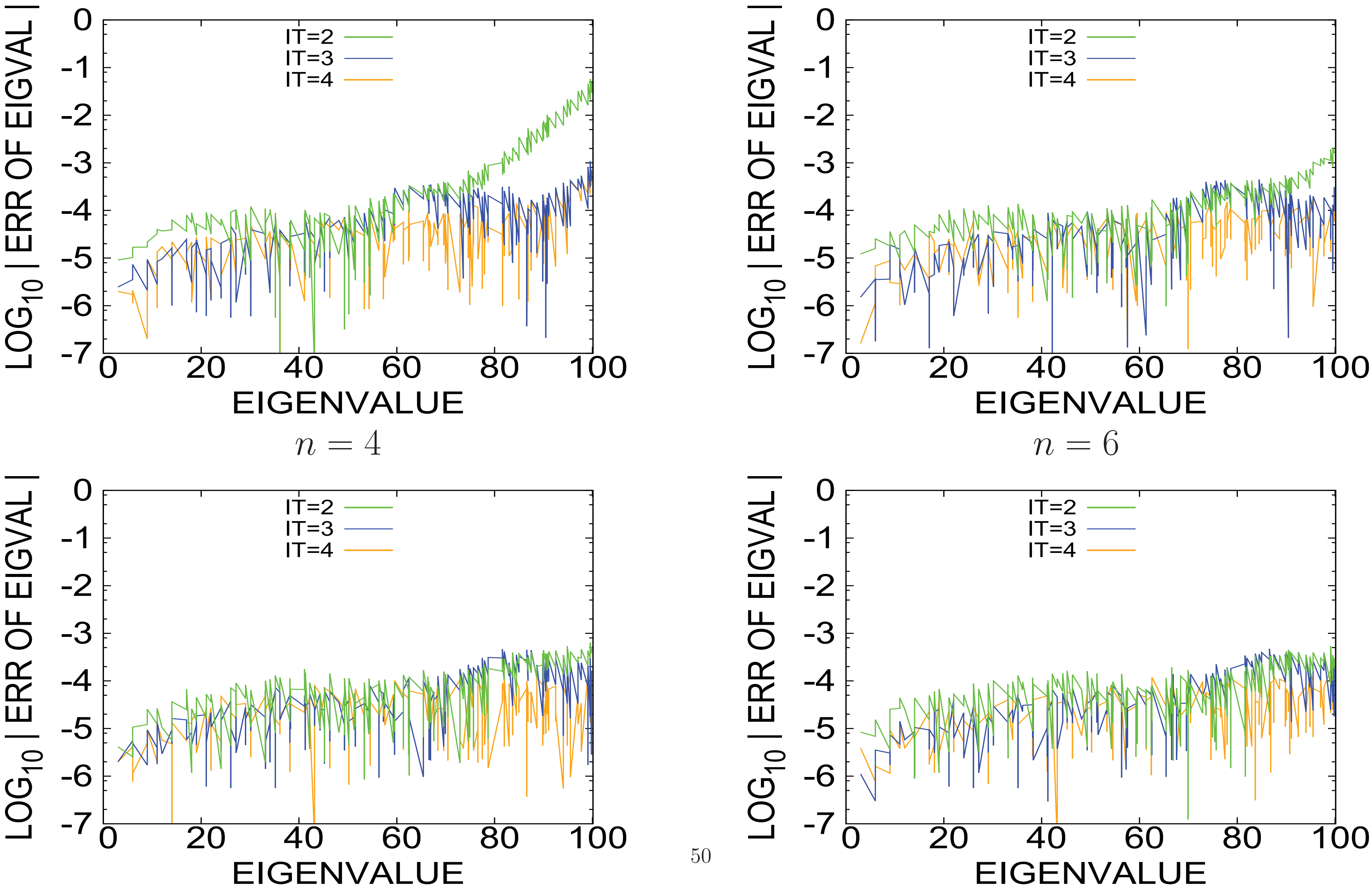
(Ex-1b): Relative Residual (D-P calculation)



$n = 4$ $n = 6$

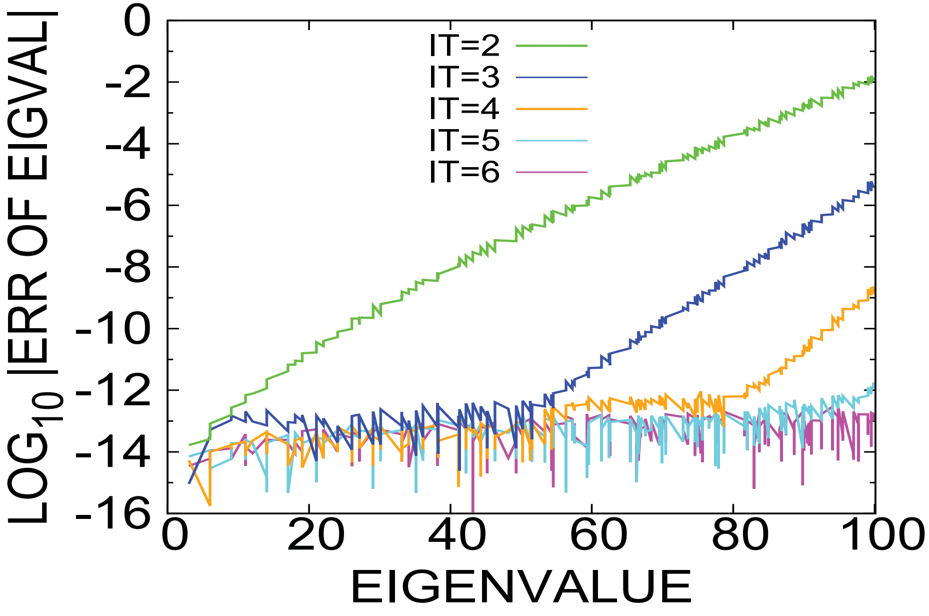
$n = 8$ $n = 10$

(Ex-1b): Error of Eigenvalue (S-P calculation)

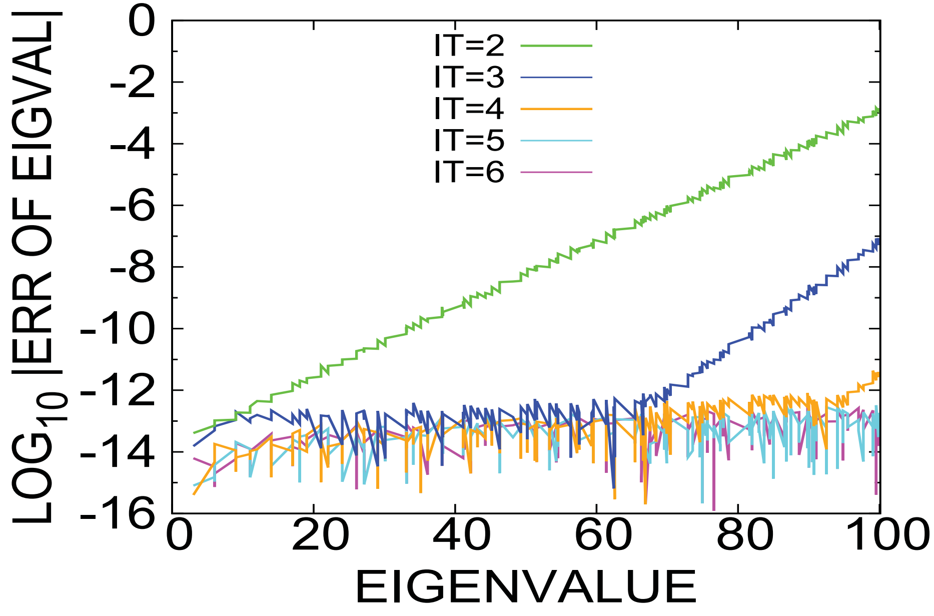


$n = 4$ $\quad$ $n = 6$ $\quad$ $n = 8$ $\quad$ $n = 10$

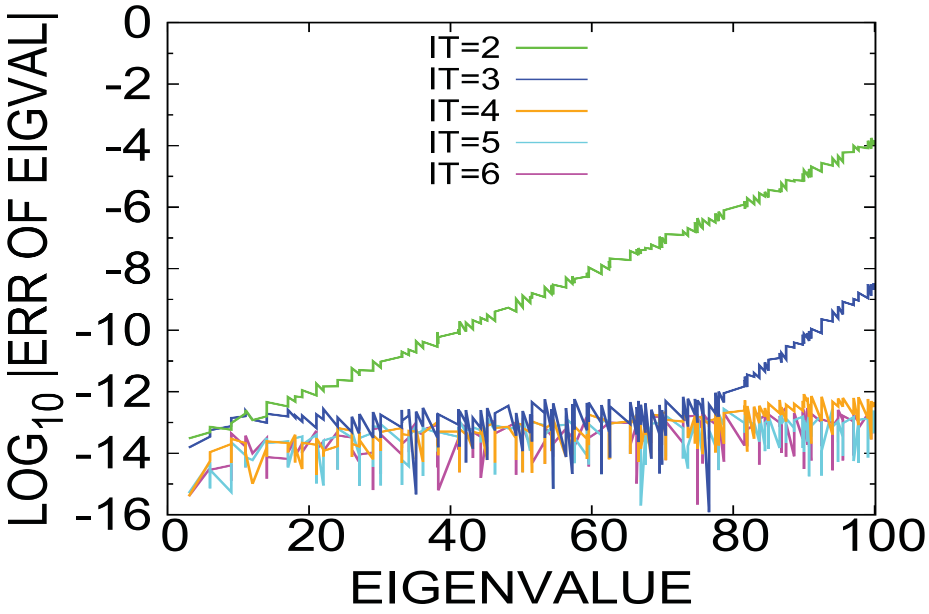
(Ex-1b): Error of Eigenvalue (D-P calculation)



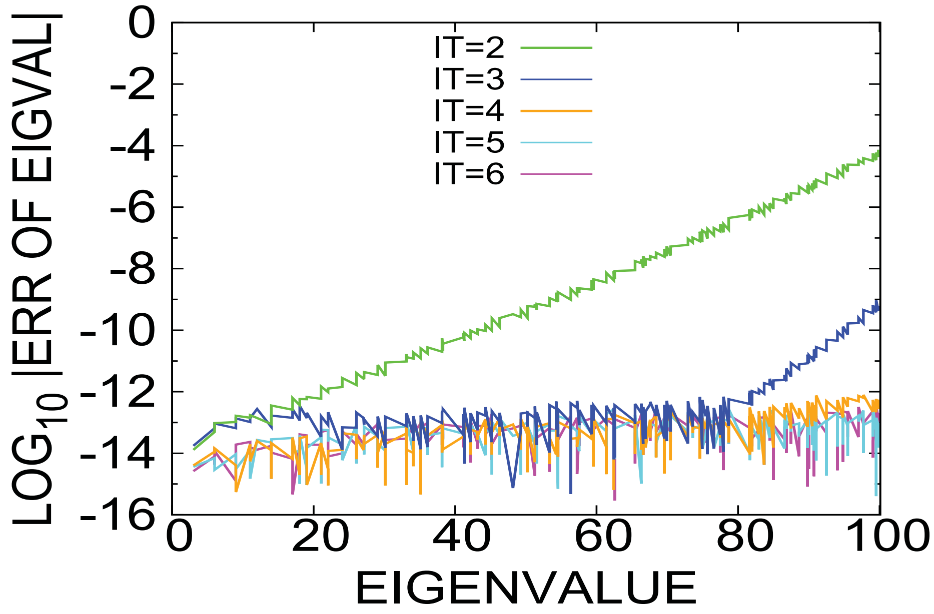
$n = 4$



$n = 6$



$n = 8$



$n = 10$

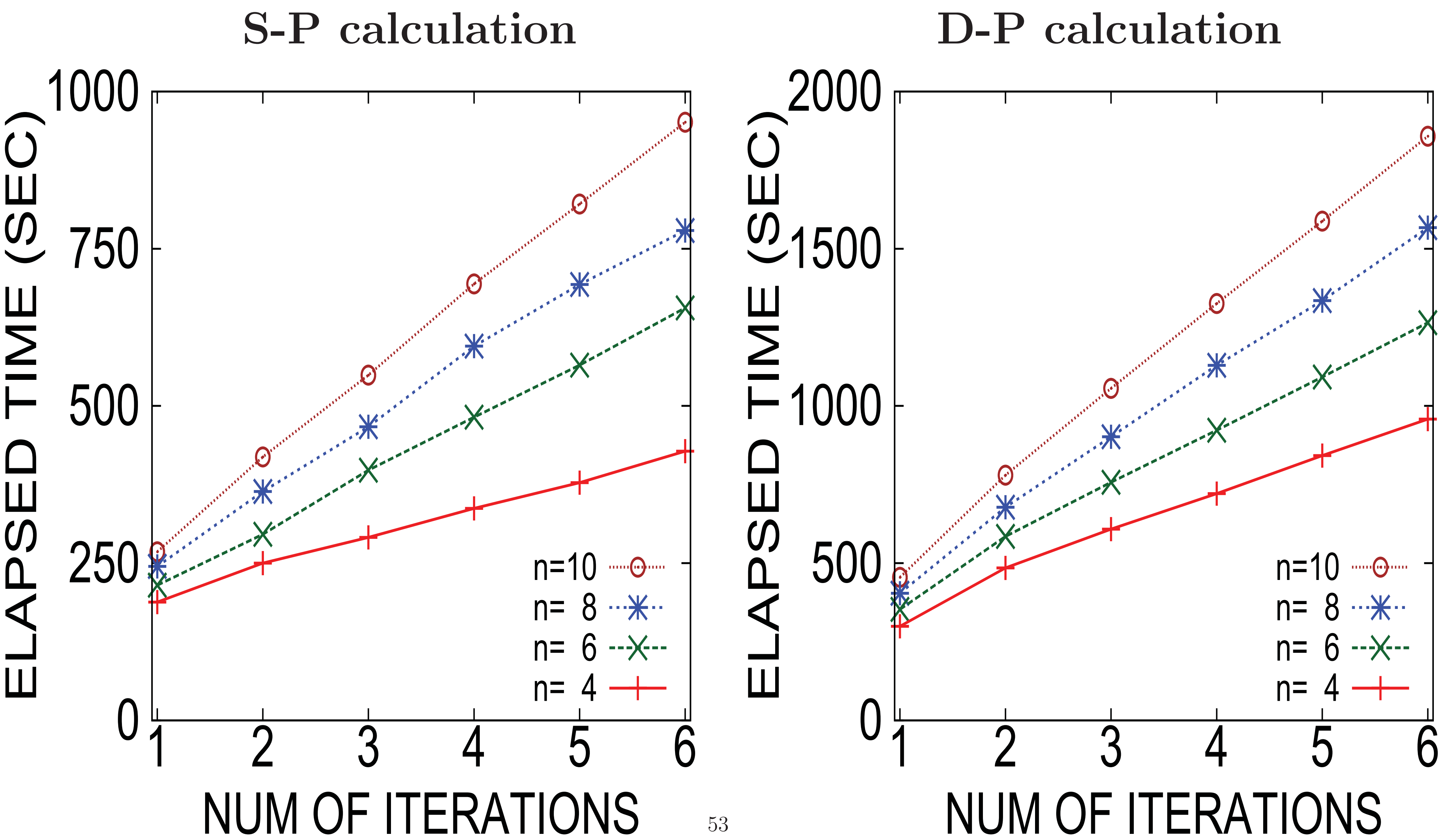
Elapsed Time in Seconds

(Ex-1b): For lower-end eigenpairs ($m = 800$ initial vectors)

IT	$n = 4$	$n = 6$	$n = 8$	$n = 10$
1	188(299)	215(353)	245(404)	268(455)
2	250(485)	296(585)	364(678)	419(780)
3	291(608)	398(757)	467(902)	549(1,056)
4	337(721)	482(923)	595(1,129)	694(1,326)
5	378(842)	565(1,092)	693(1,335)	821(1,588)
6	428(958)	656(1,265)	779(1,567)	951(1,858)

(Data in parenthesis are from D-P calculations.)

(Ex-1b, Lower-end Eigenpairs): Elapsed Time in Seconds



Ex-2b : INTERIOR EIGENPAIRS

(Ex-2b): Num of Approx Eigenpairs and Max Rel Residuals

($\mu = 1.5$, $g_{\mathtt{s}} = \mathtt{1E-5}$, $m = 1,300$, the correct num of pairs is 798).

$n = 4$

IT	# Eigenpairs	Max Rel Residual
1	<u>701</u>(<u>701</u>)	3.0E-01 (3.0E-01)
2	798(798)	2.3E-03 (2.5E-03)
3	798(798)	5.3E-05 (7.7E-06)
4	798(798)	2.2E-05 (2.1E-08)

$n = 6$

IT	# Eigenpairs	Max Rel Residual
1	<u>799</u>(<u>799</u>)	3.4E-01 (3.3E-01)
2	798(798)	2.1E-04 (2.1E-04)
3	798(798)	2.3E-05 (1.9E-07)
4	798(798)	2.2E-05 (1.5E-10)

$n = 8$

IT	# Eigenpairs	Max Rel Residual
1	<u>828</u>(<u>827</u>)	3.2E-01 (3.4E-01)
2	798(798)	8.1E-05 (6.8E-05)
3	798(798)	3.3E-05 (3.2E-08)
4	798(798)	3.2E-05 (1.6E-11)

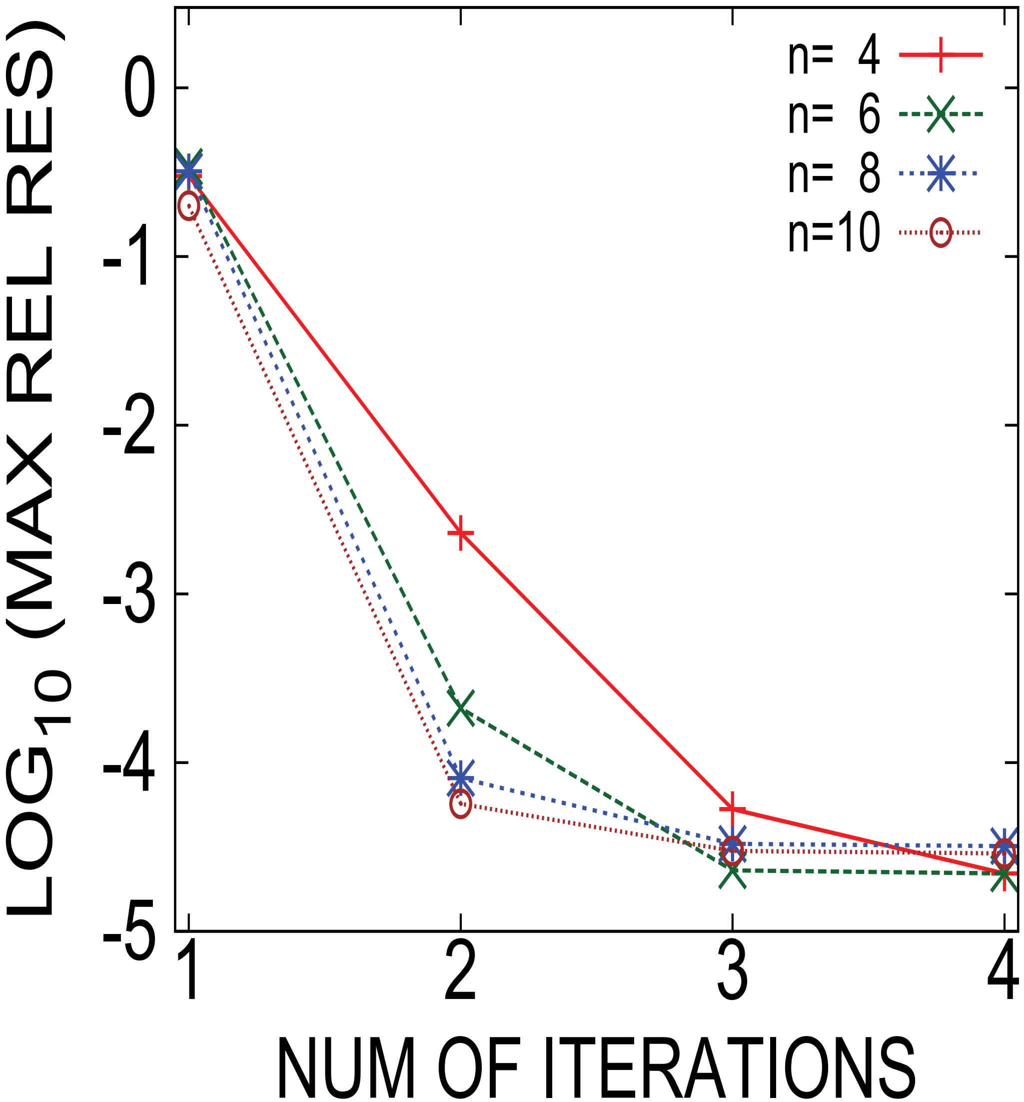
$n = 10$

IT	# Eigenpairs	Max Rel Residual
1	<u>797</u>(<u>791</u>)	2.0E-01 (2.7E-01)
2	798(798)	5.7E-05 (3.5E-05)
3	798(798)	3.0E-05 (1.3E-08)
4	798(798)	2.9E-05 (4.1E-12)

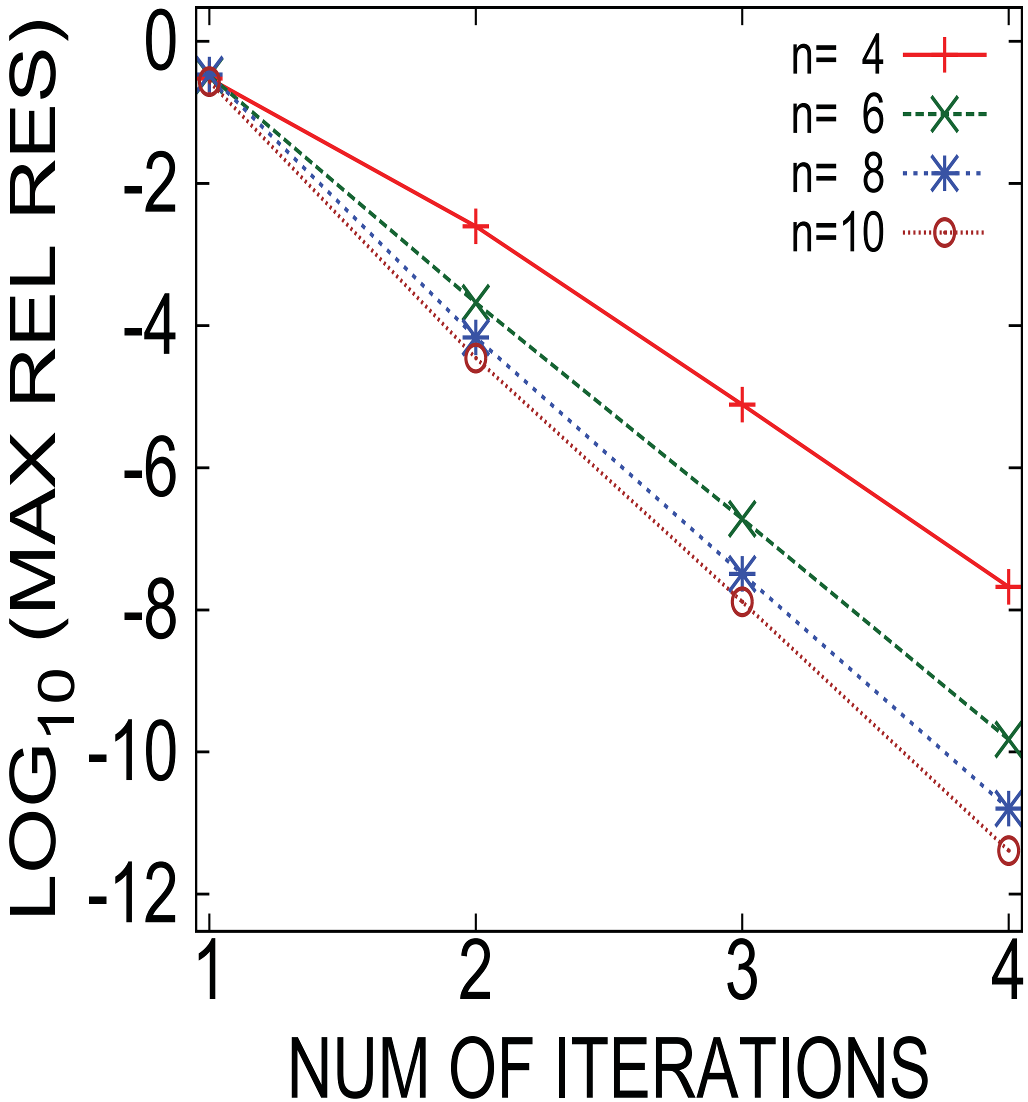
(Data in parenthesis are from D-P calculations.)

(Ex-2b, Interior Eigenpairs): Max of Relative Residuals

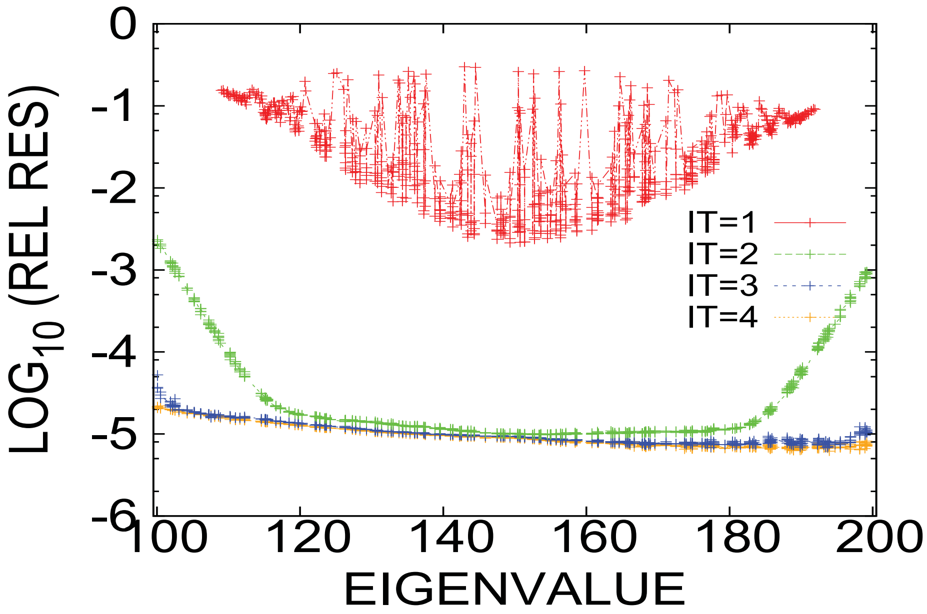
S-P calculation



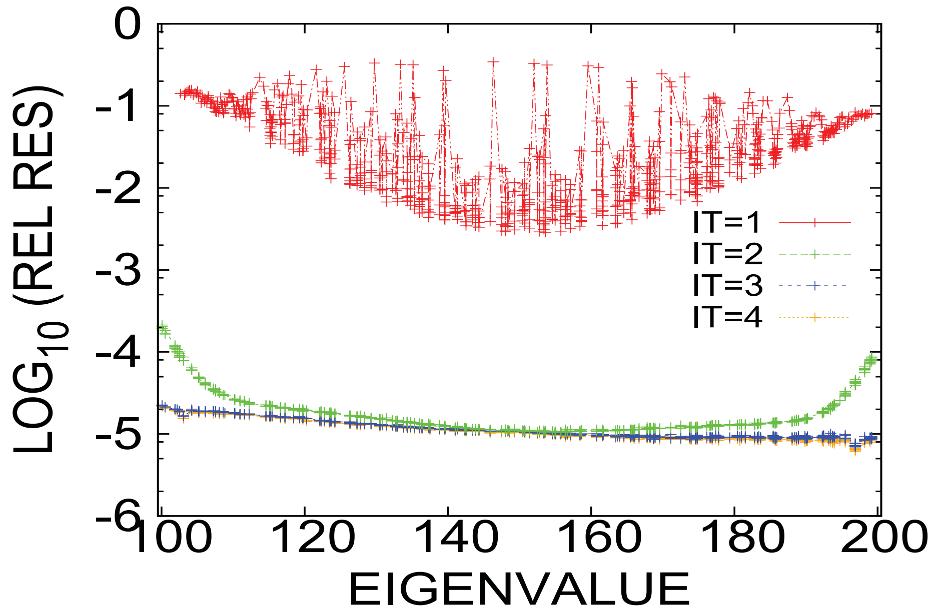
D-P calculation



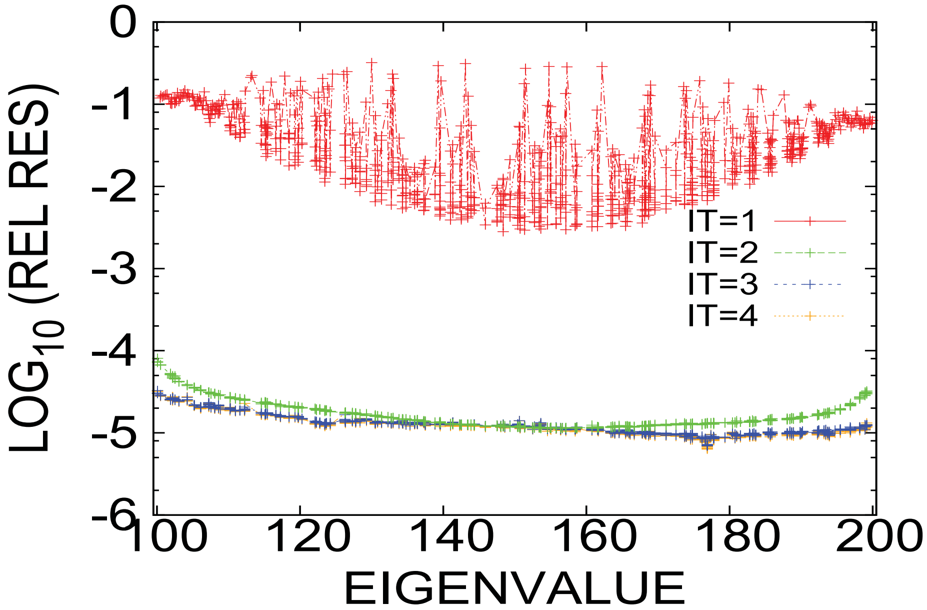
(Ex-2b): Relative Residual (S-P calculation)



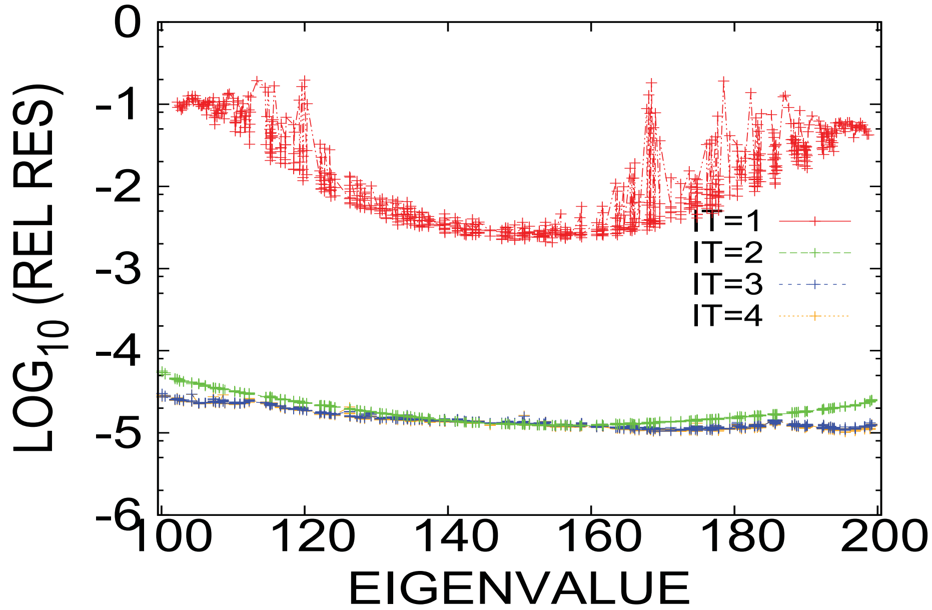
$n = 4$



$n = 6$

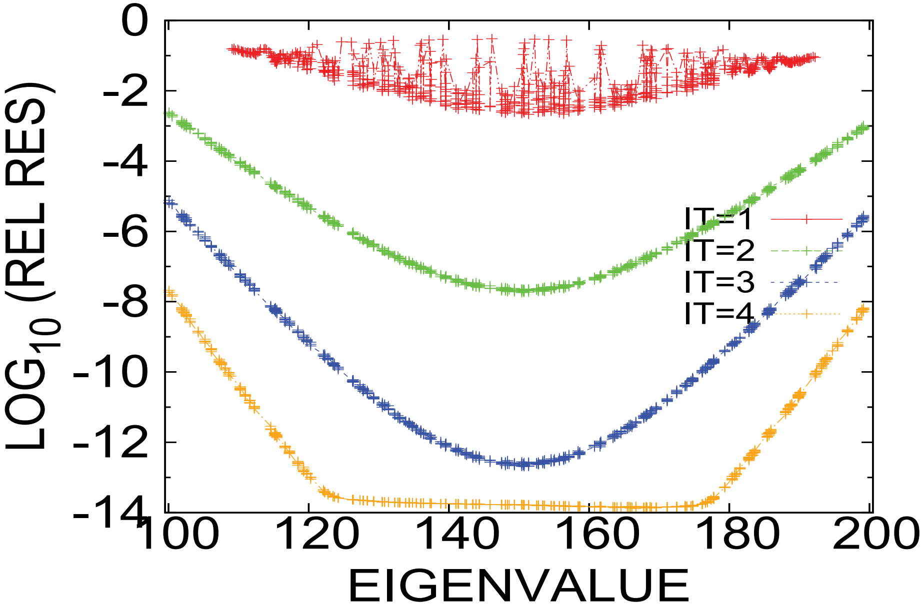


$n = 8$

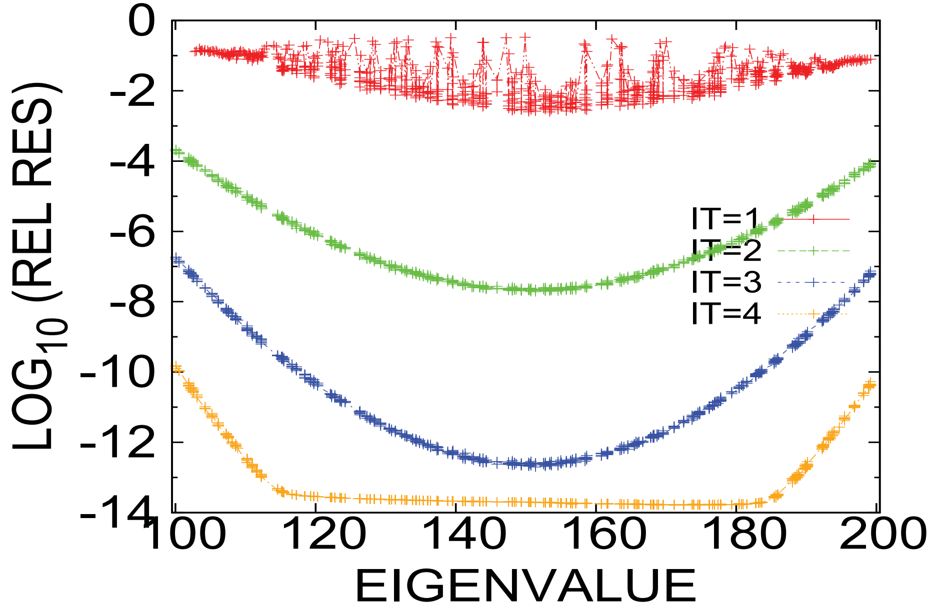


$n = 10$

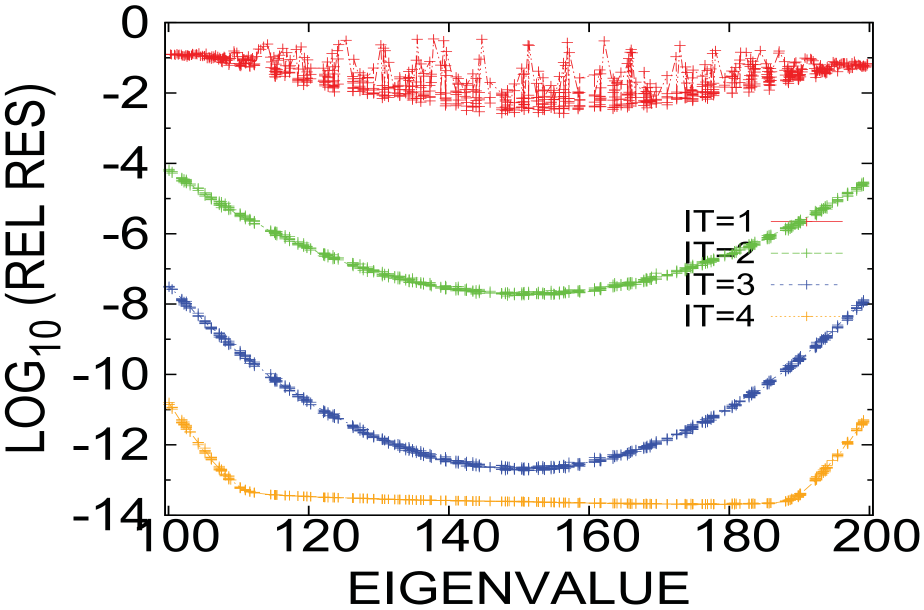
(Ex-2b): Relative Residual (D-P calculation)



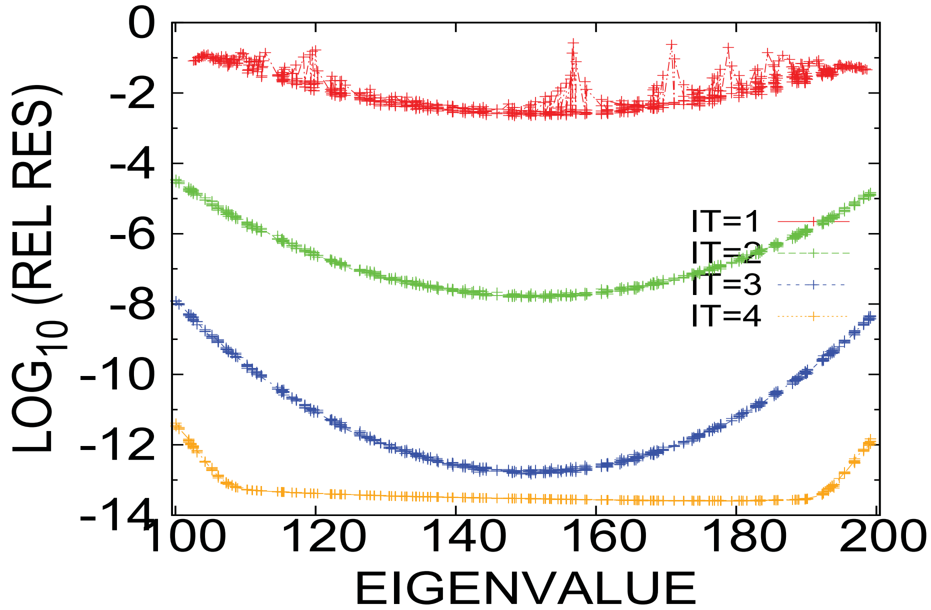
$n = 4$



$n = 6$

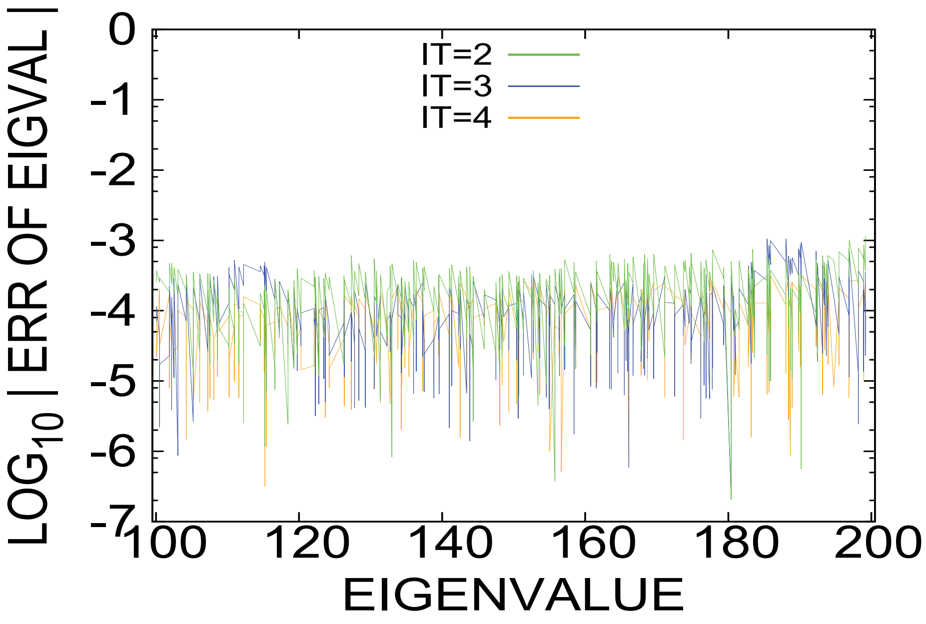


$n = 8$

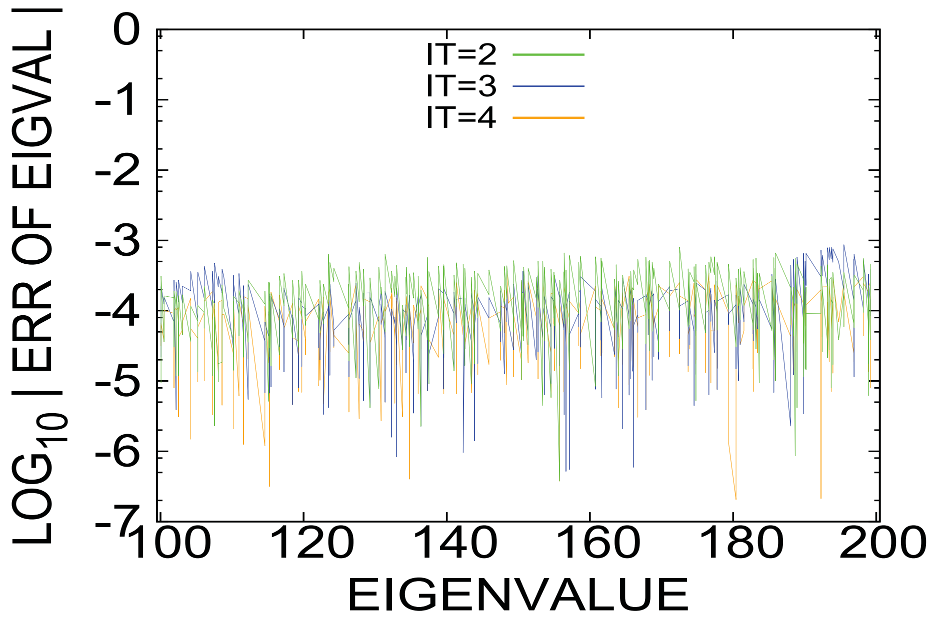


$n = 10$

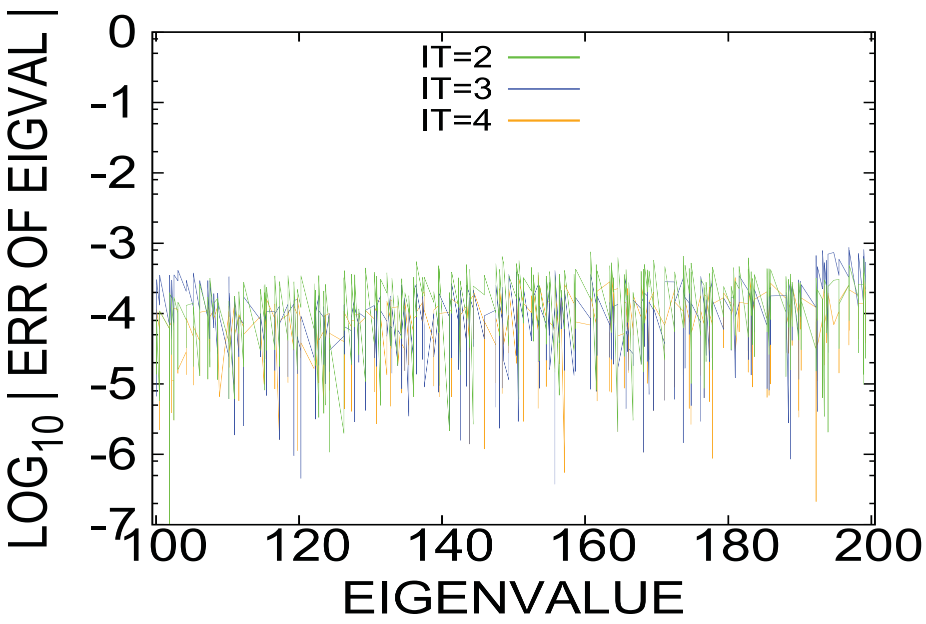
(Ex-2b): Error of Eigenvalue (S-P calculation)



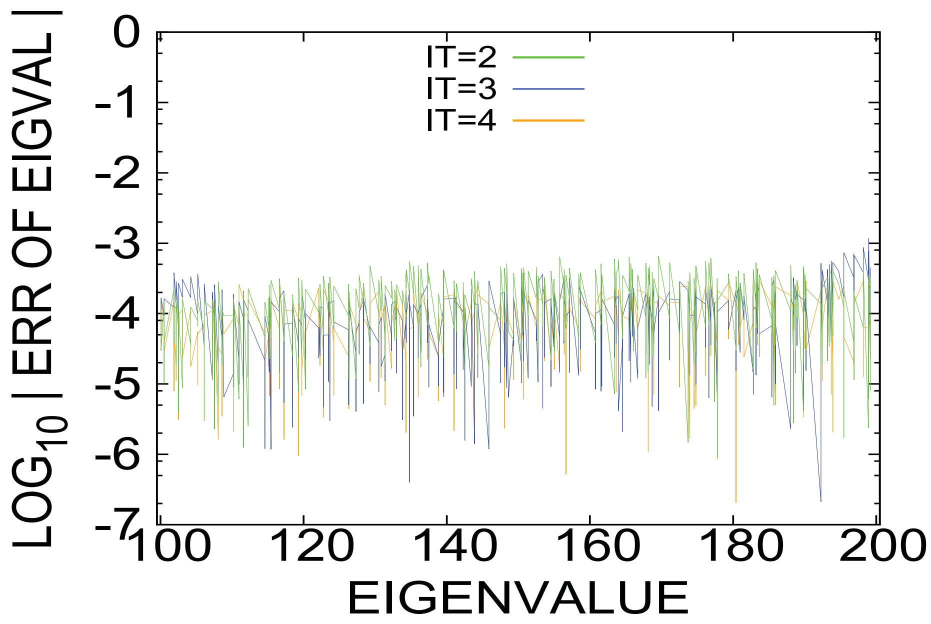
$n = 4$



$n = 6$

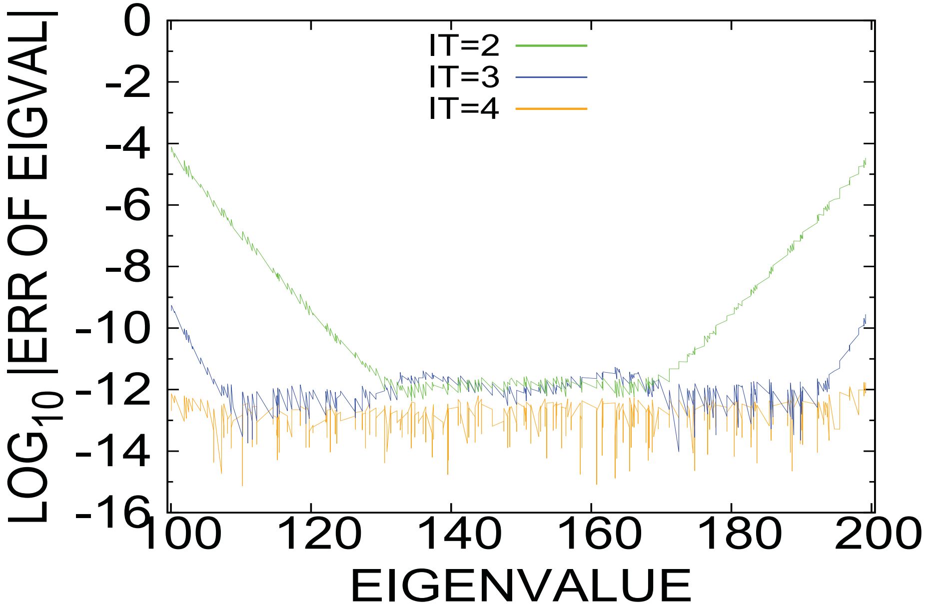


$n = 8$

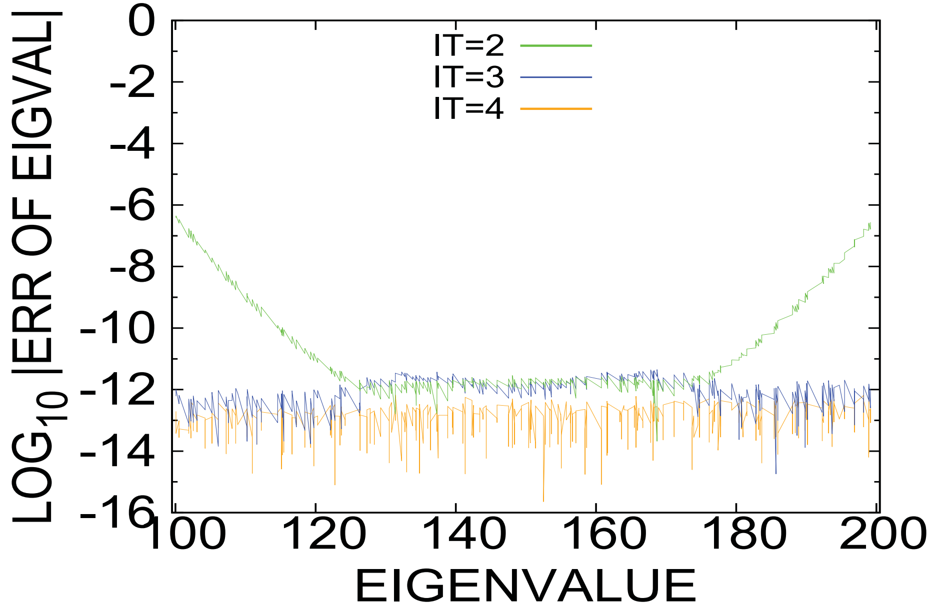


$n = 10$

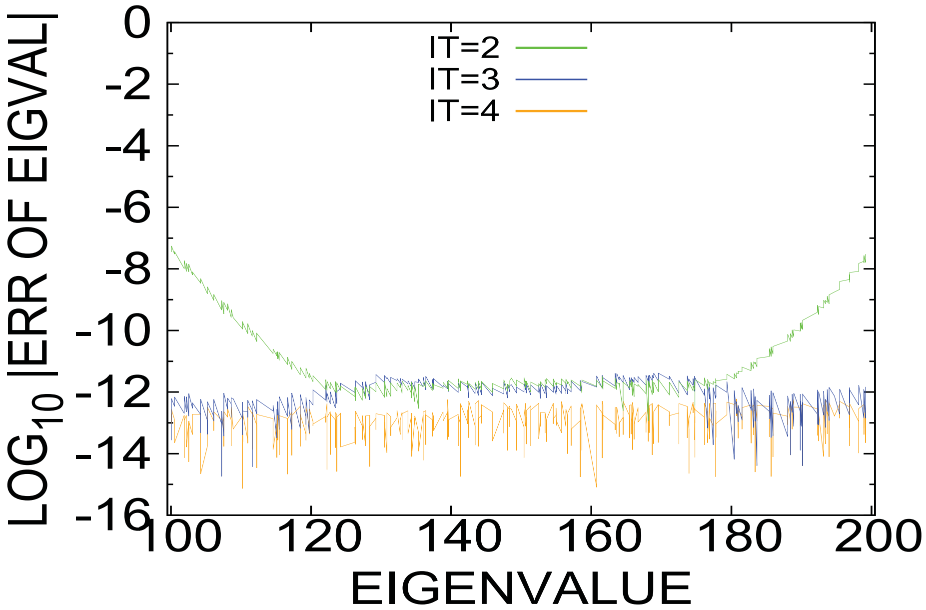
(Ex-2b): Error of Eigenvalue (D-P calculation)



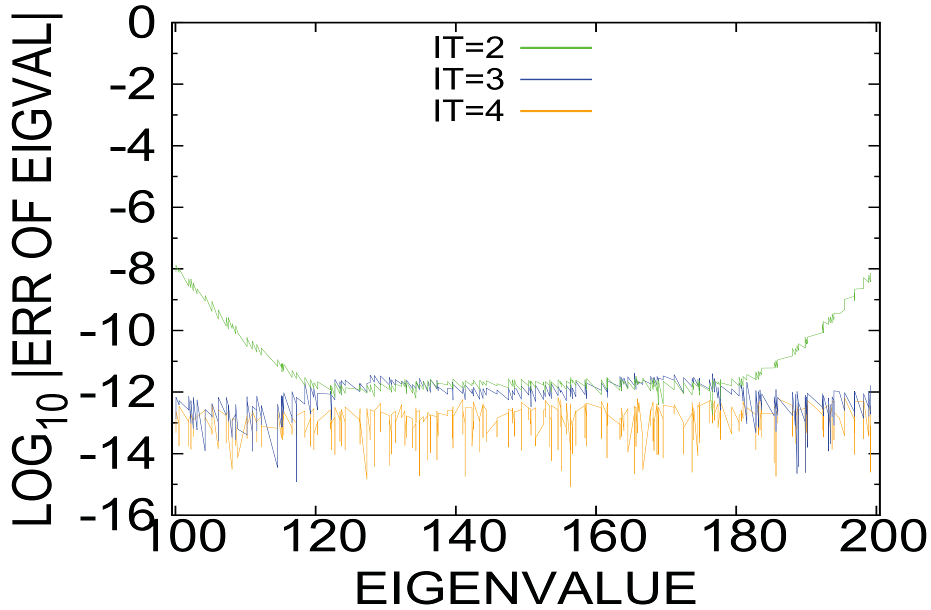
$n = 4$



$n = 6$



$n = 8$



$n = 10$

Elapsed Time in Seconds

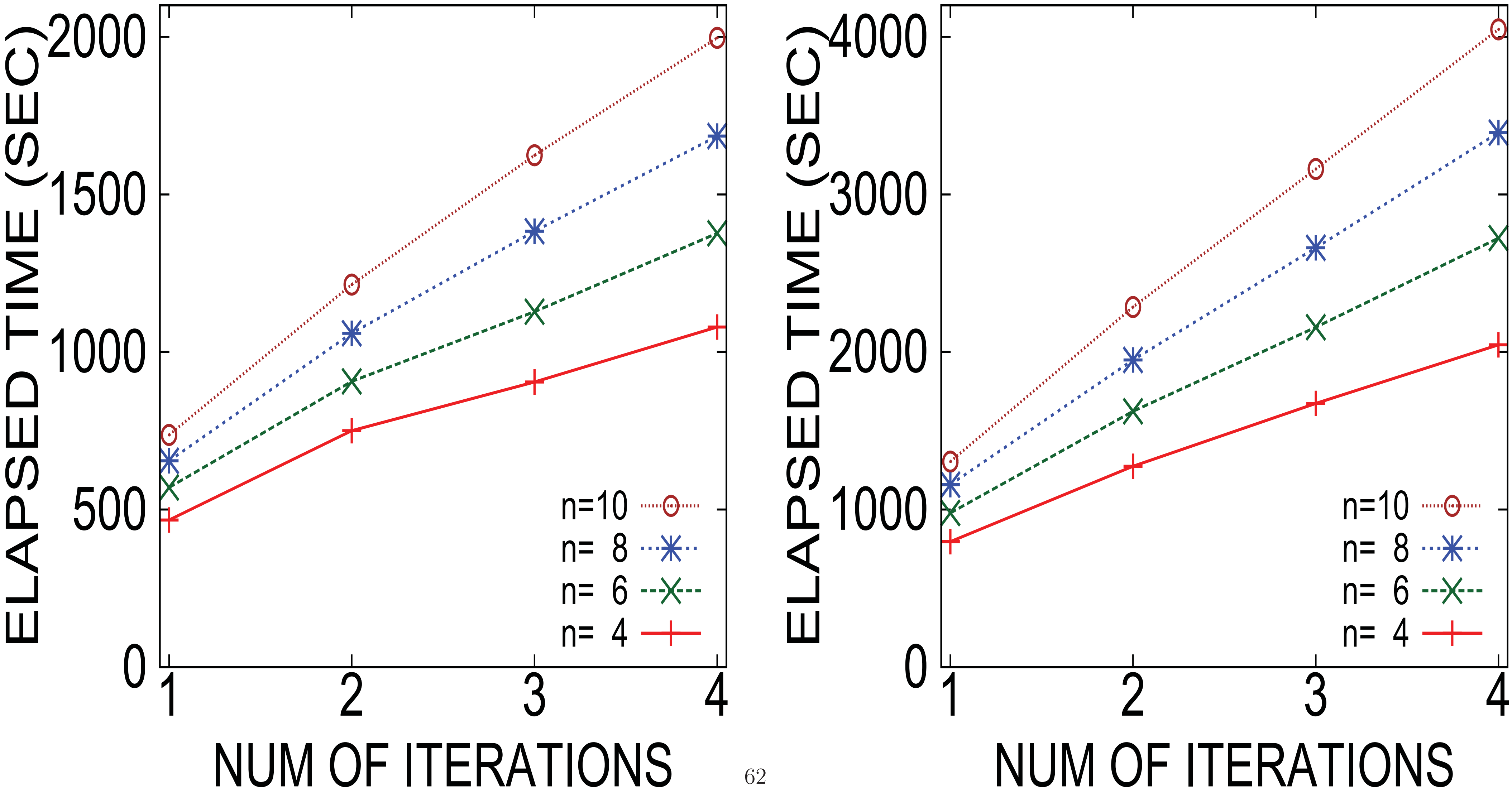
(Ex-2b): For interior eigenpairs ($m = 1,300$ initial vectors)

IT	$n = 4$	$n = 6$	$n = 8$	$n = 10$
1	467(796)	570(979)	655(1,158)	737(1,304)
2	750(1,275)	907(1,624)	1,059(1,949)	1,214(2,285)
3	905(1,674)	1,128(2,157)	1,383(2,661)	1,624(3,161)
4	1,079(2,046)	1,377(2,723)	1,685(3,392)	1,997(4,047)

(Data in parenthesis are from D-P calculations.)

(Ex-2b, Interior Eigenpairs): Elapsed Time in Seconds

S-P calculation **D-P calculation**



THE END OF APPENDIX