Implementations of the Levin-Weniger convergence accelerator and applications to problems in physics

Ignacio Porras, Francisco Cordobés-Aguilar

Departamento de Física Atómica, Molecular y Nuclear

Universidad de Granada

Luminy 09 Conference

Outline:

- Introduction.

Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.

Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.

Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.

Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.
- Generalizing Čížek et al's generalization of Levin-Weniger transformations.

Outline:

- Introduction.
- A new remainder for the generalized Levin transformation.
- Attempts to improve stability.
- Series appearing in few-electron integrals.
- Generalizing Čížek et al's generalization of Levin-Weniger transformations.
- Conclusions.

Introduction:

- Convergence acceleration is an important problem in many problems in physics.

Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.

Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.

Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.
- Large basis sets: necessity of reducing computing time.

Introduction:

- Convergence acceleration is an important problem in many problems in physics.
- Variational calculations in atomic physics: multiple series for the calculation of each matrix element of the Hamiltonian.
- High precision is demanded.
- Large basis sets: necessity of reducing computing time.
- Crucial problems: negative ions.

Generalized Levin transformed reviewed by Weniger

- For a series $S = \sum_{i=0}^{\infty} a_i$, where $S_n = \sum_{i=0}^{n} a_i$, for which we assume

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)^j}$$

Generalized Levin transformed reviewed by Weniger

- For a series $S = \sum_{i=0}^{\infty} a_i$, where $S_n = \sum_{i=0}^{n} a_i$, for which we assume

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)^j}$$

- Then, multiplying by $(n+\beta)^{k-1}$ both sides:

$$(n+\beta)^{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } \quad k-1$$

Generalized Levin transformed reviewed by Weniger

- For a series $S = \sum_{i=0}^{\infty} a_i$, where $S_n = \sum_{i=0}^{n} a_i$, for which we assume

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)^j}$$

- Then, multiplying by $(n+\beta)^{k-1}$ both sides:

$$(n+\beta)^{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } \quad k-1$$

- And applying the k-th power of the difference operator Δ^k:

$$S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{S_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{1}{\omega_{n+j}}}$$

E.J. Weniger, *Comp. Phys. Rep.* **10**, 189 (1989).

A new remainder for g-Levin transformation

- Levin's u-transformation: $\omega_n = na_n$ or $\omega_n = (n+\beta)a_n$ (inspired in integrals)

A new remainder for g-Levin transformation

- Levin's u-transformation: $\omega_n = n a_n$ or $\omega_n = (n+\beta) a_n$ (inspired in integrals)
- Formal obtention of a remainder for series for which $a_n \sim n^{-\alpha}$, using Euler-McLaurin sum rule:

$$\sum_{i=n}^{\infty} a_i = \int_n^{\infty} f(x)\, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m$$

where

A new remainder for g-Levin transformation

- Levin's u-transformation: $\omega_n = n a_n$ or $\omega_n = (n+\beta) a_n$ (inspired in integrals)
- Formal obtention of a remainder for series for which $a_n \sim n^{-\alpha}$, using Euler-McLaurin sum rule:

$$\sum_{i=n}^{\infty} a_i = \int_n^{\infty} f(x)\,dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m$$

where

- $f(x)$ verifies $f(i) = a_i$ for $i = n, n+1, \ldots,$

A new remainder for g-Levin transformation

- Levin's u-transformation: $\omega_n = n a_n$ or $\omega_n = (n+\beta) a_n$ (inspired in integrals)
- Formal obtention of a remainder for series for which $a_n \sim n^{-\alpha}$, using Euler-McLaurin sum rule:

$$\sum_{i=n}^{\infty} a_i = \int_n^{\infty} f(x)\, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m$$

where

- $f(x)$ verifies $f(i) = a_i$ for $i = n, n+1, \ldots,$
- B_n denote the Bernouilli numbers,

A new remainder for g-Levin transformation

- Levin's u-transformation: $\omega_n = n a_n$ or $\omega_n = (n+\beta) a_n$ (inspired in integrals)
- Formal obtention of a remainder for series for which $a_n \sim n^{-\alpha}$, using Euler-McLaurin sum rule:

$$\sum_{i=n}^{\infty} a_i = \int_n^{\infty} f(x)\, dx + \frac{1}{2} f(n) - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} f^{(2k-1)}(N) + E_m$$

  where
  - $f(x)$ verifies $f(i) = a_i$ for $i = n, n+1, \ldots,$
  - B_n denote the Bernouilli numbers,
  - and E_m is a remainder term.

- If n is large enough and $f(x) \sim \frac{C}{x^\alpha}$:

$$\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1}\frac{1}{n^{\alpha-1}} + \frac{C}{2}\frac{1}{n^\alpha} + \sum_{k=1}^{m} \frac{B_{2k} C(\alpha)_{2k-1}}{(2k)!}\frac{1}{n^{\alpha+2k-1}} + E_m$$

- If n is large enough and $f(x) \sim \frac{C}{x^\alpha}$:

$$\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1}\frac{1}{n^{\alpha-1}} + \frac{C}{2}\frac{1}{n^\alpha} + \sum_{k=1}^{m} \frac{B_{2k} C(\alpha)_{2k-1}}{(2k)!}\frac{1}{n^{\alpha+2k-1}} + E_m$$

- We applicate this result to the sum:

$$S = \sum_{i=0}^{\infty} a_i = \sum_{i=0}^{n-1} a_i + \sum_{i=n}^{\infty} a_i = S_{n-1} + \sum_{i=n}^{\infty} a_i$$

up to k terms, for the second sum, including for convenience the missing terms ($1/n^{\alpha+2k}$).

- If n is large enough and $f(x) \sim \frac{C}{x^\alpha}$:

$$\sum_{i=n}^{\infty} a_i = \frac{C}{\alpha - 1}\frac{1}{n^{\alpha-1}} + \frac{C}{2}\frac{1}{n^\alpha} + \sum_{k=1}^{m} \frac{B_{2k}C(\alpha)_{2k-1}}{(2k)!}\frac{1}{n^{\alpha+2k-1}} + E_m$$

- We applicate this result to the sum:

$$S = \sum_{i=0}^{\infty} a_i = \sum_{i=0}^{n-1} a_i + \sum_{i=n}^{\infty} a_i = S_{n-1} + \sum_{i=n}^{\infty} a_i$$

up to k terms, for the second sum, including for convenience the missing terms ($1/n^{\alpha+2k}$).

- We obtain and estimator for S that will be denoted by Q_0.

$$S_{n-1} = Q_0 + \frac{Q_1}{n^{\alpha-1}} + \frac{Q_2}{n^\alpha} + \cdots + \frac{Q_k}{n^{\alpha+k-2}}$$

- Applying this result for $n, \ldots n+k$, we find a system of equations than can be solved for Q_0:

$$Q_0^{(\alpha)}(n,k) = \frac{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2} S_{n+j}}{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2}},$$

- Applying this result for $n, \ldots n+k$, we find a system of equations than can be solved for Q_0:

$$Q_0^{(\alpha)}(n,k) = \frac{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2} S_{n+j}}{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2}},$$

- Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n+1)^{-\alpha+1}$, which is equivalent to u-transform in the large n-limit.

- Applying this result for $n, \ldots n+k$, we find a system of equations than can be solved for Q_0:

$$Q_0^{(\alpha)}(n,k) = \frac{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2} S_{n+j}}{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2}},$$

- Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n+1)^{-\alpha+1}$, which is equivalent to u-transform in the large n-limit.
- For n not large, differences appear.

- Applying this result for $n, \ldots n+k$, we find a system of equations than can be solved for Q_0:

$$Q_0^{(\alpha)}(n,k) = \frac{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2} S_{n+j}}{\displaystyle\sum_{j=0}^{k} \frac{(-1)^j}{j!(k-j)!}(n+j+1)^{k+\alpha-2}},$$

- Equal to g-Levin formula for $\beta = 1$ and $\omega_n = (n+1)^{-\alpha+1}$, which is equivalent to u-transform in the large n-limit.
- For n not large, differences appear.
- $\alpha = 2$ leads to Richardson's convergence accelerator.

Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when k increases, getting worse as n increases.

Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when k increases, getting worse as n increases.
- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between S_{n+j} values, for different j, fixed n.

Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when k increases, getting worse as n increases.
- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between S_{n+j} values, for different j, fixed n.
- Summing and substracting S_n leads to:

$$S = S_n + \frac{\displaystyle\sum_{j=1}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{P_{n,j}}{\omega_{n+j}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{1}{\omega_{n+j}}}$$

Unstability problems:

- Alternating sums of close values in numerator and denominator. Problems when k increases, getting worse as n increases.
- Attempt to improve stability: we assume that differences in the values $P_{n,j} = S_{n+j} - S_n = \sum_{i=n+1}^{n+j} a_i$ are greater than differences between S_{n+j} values, for different j, fixed n.
- Summing and substracting S_n leads to:

$$S = S_n + \frac{\displaystyle\sum_{j=1}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{P_{n,j}}{\omega_{n+j}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)^{k-1}}{(n+k+\beta)^{k-1}} \frac{1}{\omega_{n+j}}}$$

- Čížek, Zamastil and Skála obtained an accelerator in terms of $P_{n,j}$ *J. Math. Phys.*,**44** 962 (2003).

Test 1:

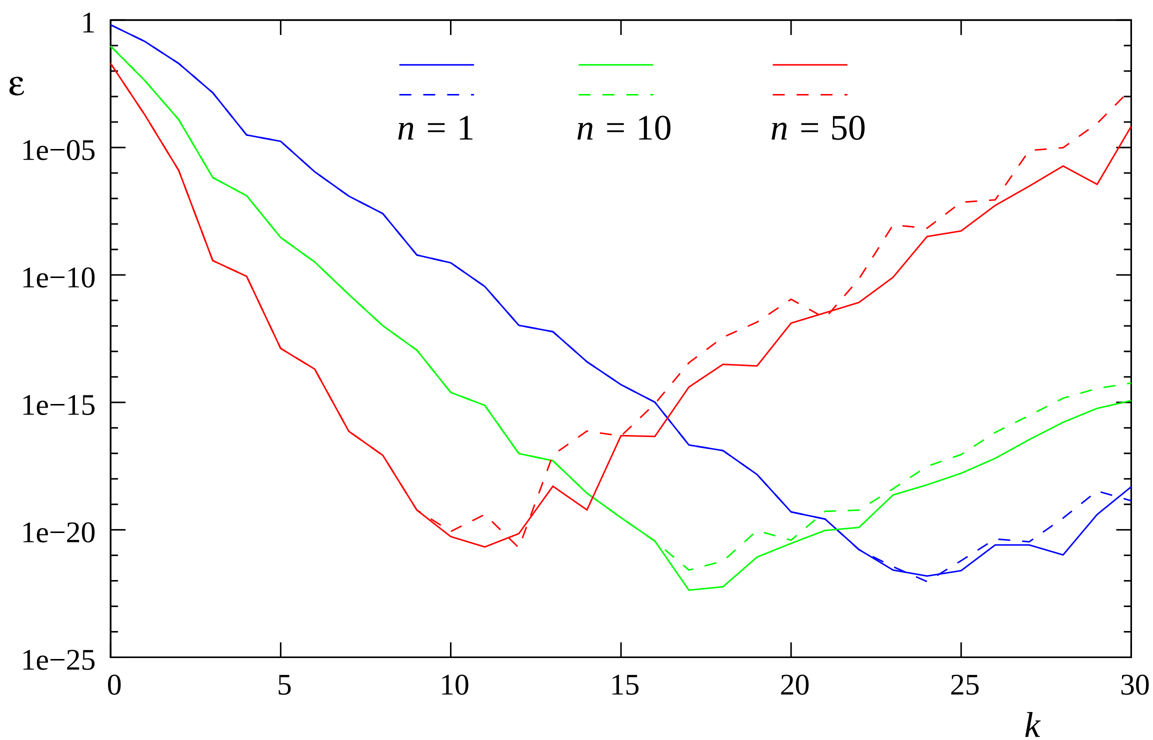
- $S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6}$

Test 1:

- $$S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6}$$
- For this case, Richardson, u-Levin and Q_0 are equivalent.

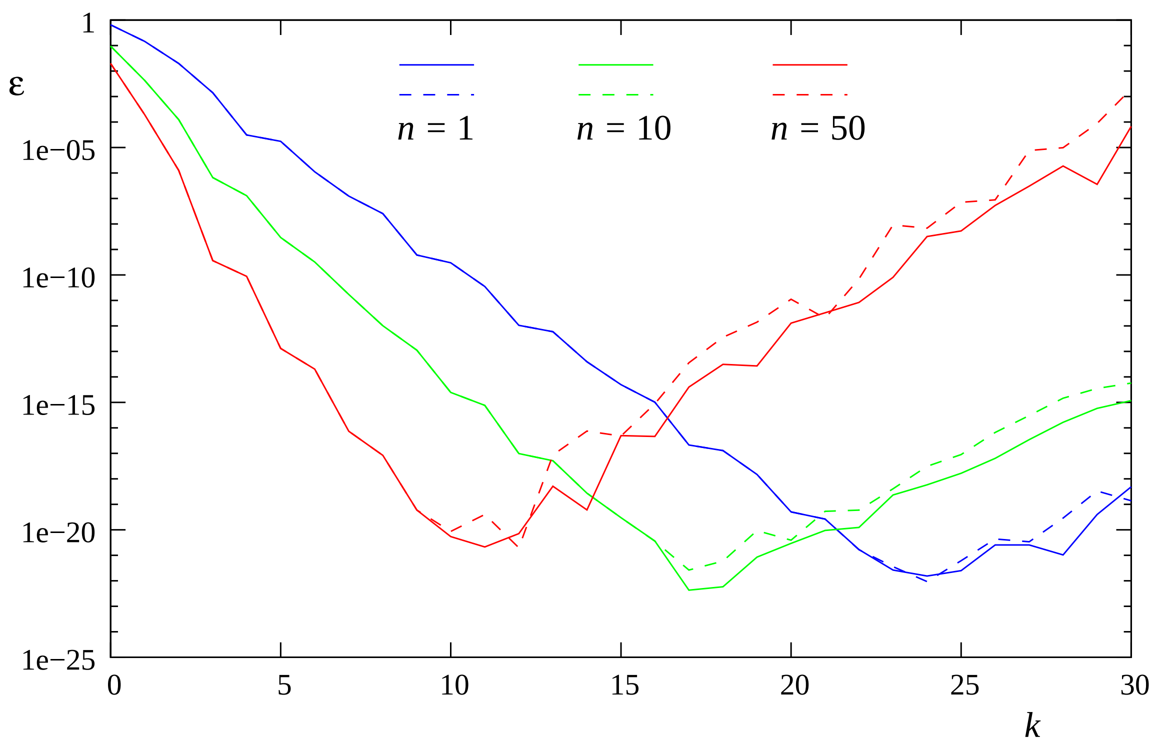
Test 1:

- $S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6}$
- For this case, Richardson, u-Levin and Q_0 are equivalent.
- ϵ: relative error (solid lines: with $P_{n,j}$, dashed lines: with S_{n+j})



Test 1:

- $S = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6}$
- For this case, Richardson, u-Levin and Q_0 are equivalent.
- ϵ: relative error (solid lines: with $P_{n,j}$, dashed lines: with S_{n+j})



- From now on, starting index $n = 1$, unless otherwise stated.

Test 2:

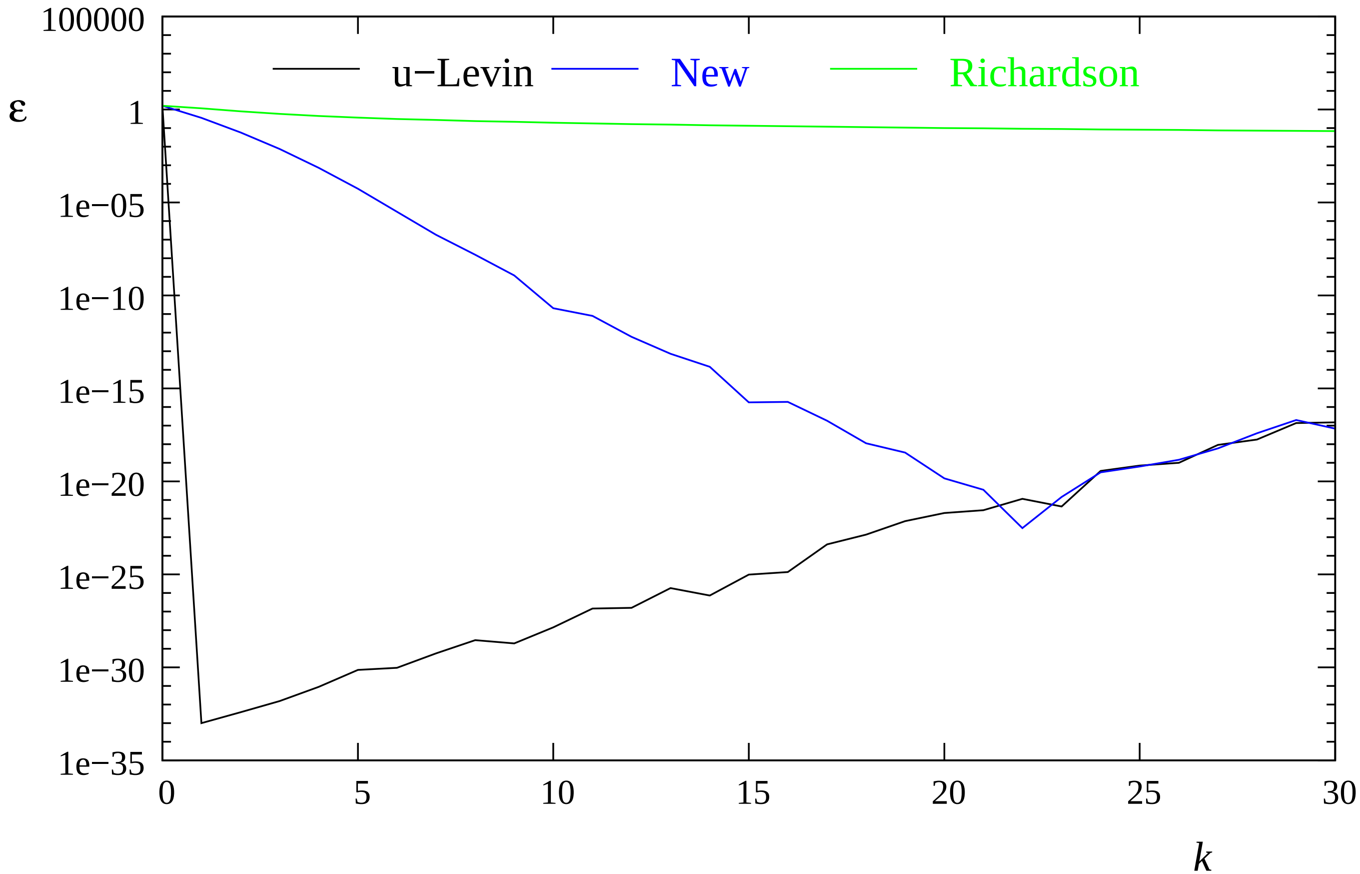
- $${}_2F_1(1,1,5/2,1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3$$

Test 2:

- $$_2F_1(1,1,5/2,1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3$$
- $a_n \sim n^{-3/2}$, $\alpha = 3/2$. u-Levin exact for this series.

Test 2:

- $$_2F_1(1,1,5/2,1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3$$
- $a_n \sim n^{-3/2}$, $\alpha = 3/2$. u-Levin exact for this series.



-

Test 3:

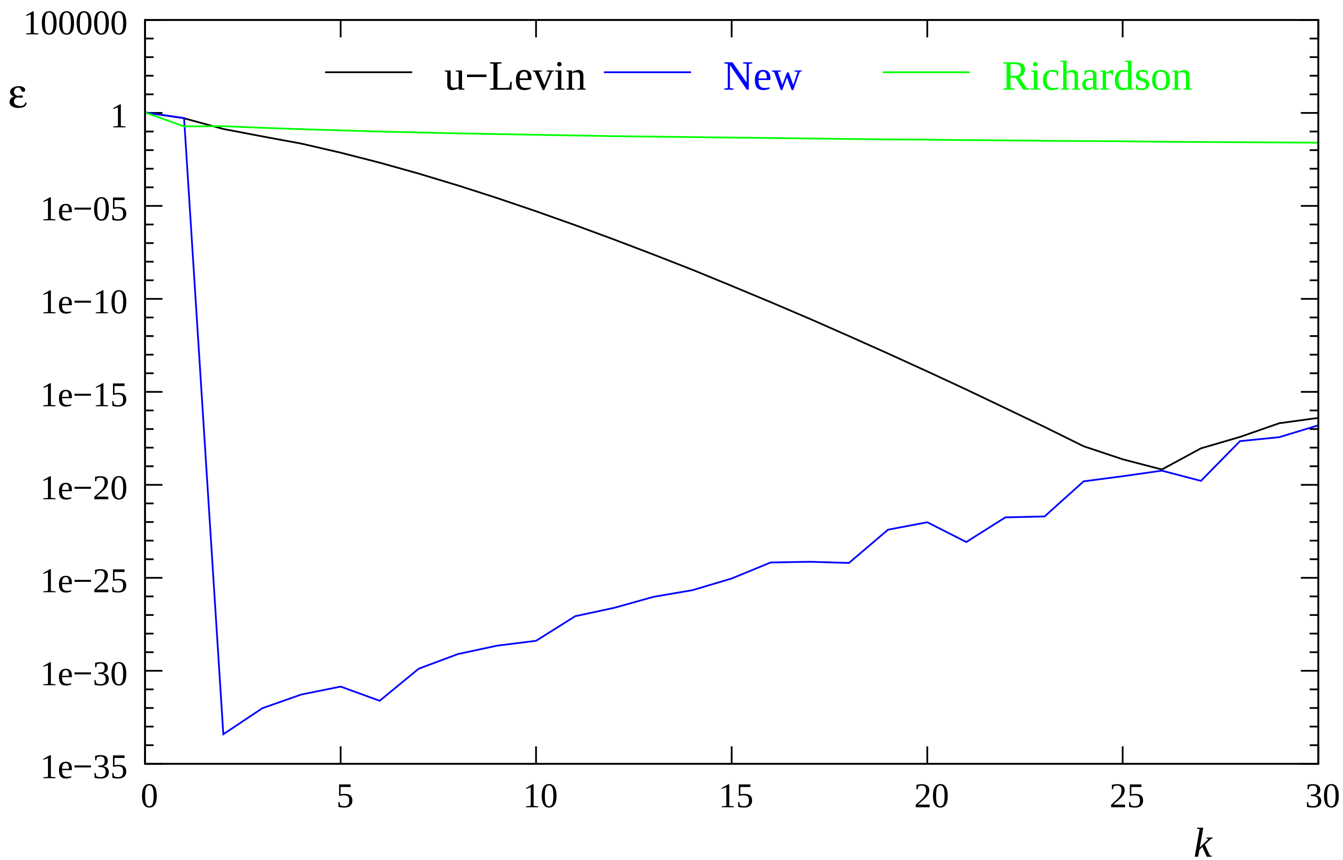
- $S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left(1 + \frac{1}{n}\right) - \frac{1}{\sqrt{n+1}} \left(1 + \frac{1}{n+1}\right) = 2$

Test 3:

- $S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left(1 + \frac{1}{n}\right) - \frac{1}{\sqrt{n+1}} \left(1 + \frac{1}{n+1}\right) = 2$
- $a_n \sim n^{-3/2}$, $Q_0^{3/2}$ is exact.

Test 3:

- $S = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left(1 + \frac{1}{n}\right) - \frac{1}{\sqrt{n+1}} \left(1 + \frac{1}{n+1}\right) = 2$
- $a_n \sim n^{-3/2}$, $Q_0^{3/2}$ is exact.



-

Test 4:

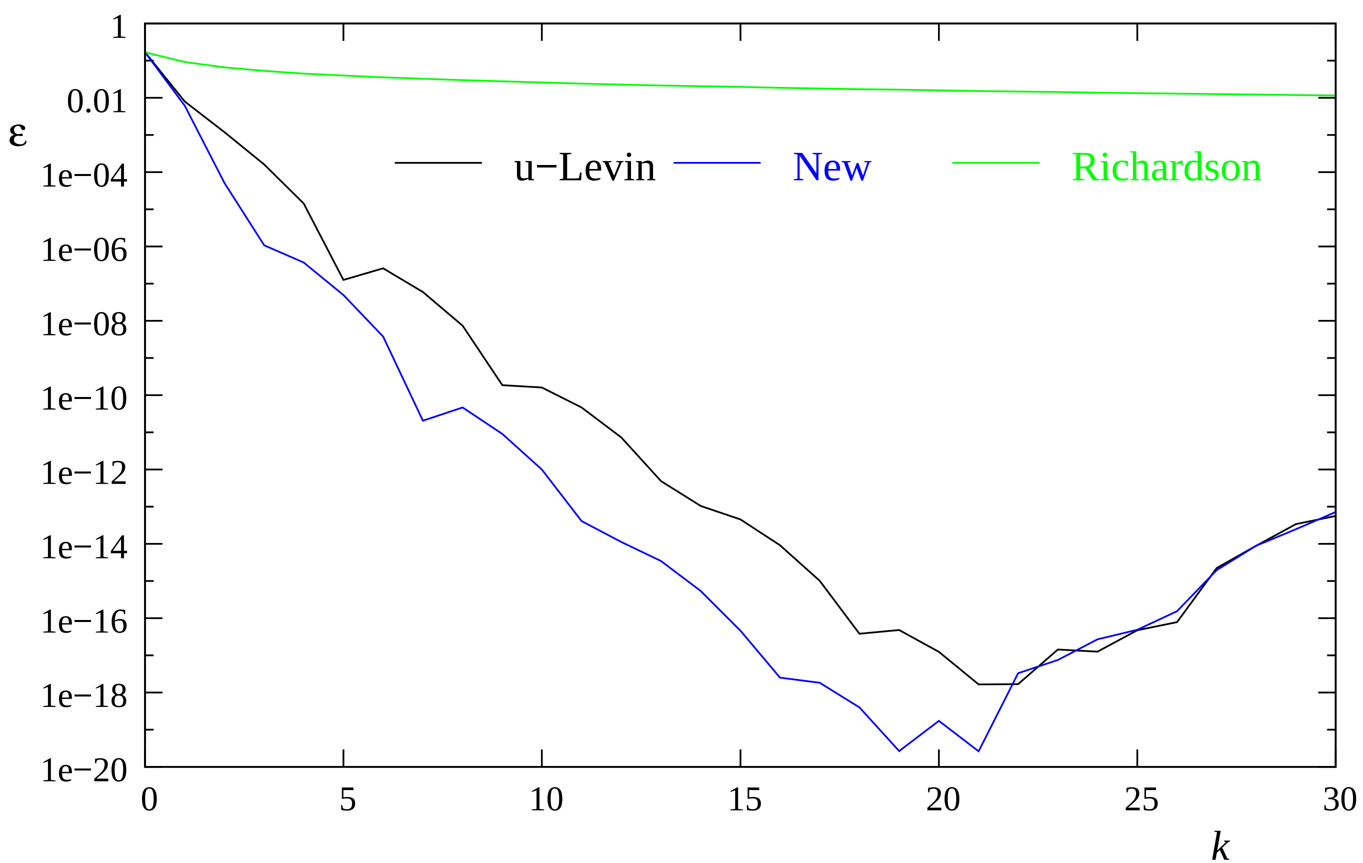
- $\frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_{m-1/2}(z) \frac{1}{2^m m!}$

Test 4:

- $\frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_{m-1/2}(z) \frac{1}{2^m m!}$
- For $z = 1$: $1 = e^{-1} \left[1 + \frac{1}{2} \sum_{n=0}^{\infty} M(-n; -2n; 2) \frac{(1/2)_n}{(n+1)!} \right]$; $a_n \sim n^{-3/2}$.

Test 4:

- $\frac{1}{z} = \sum_{m=0}^{\infty} \hat{k}_{m-1/2}(z) \frac{1}{2^m m!}$
- For $z = 1$: $1 = e^{-1} \left[1 + \frac{1}{2} \sum_{n=0}^{\infty} M(-n; -2n; 2) \frac{(1/2)_n}{(n+1)!} \right]$; $a_n \sim n^{-3/2}$.



Calculations with arbitrary precision:

- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).

Calculations with arbitrary precision:

- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).
- L. Fousse, G. Hanrot, V. Lefevre, P. Pélissier and P. Zimmermann, *ACM Transactions on Mathematical Software*, **33**, 13:1-13:15 (2007).

Calculations with arbitrary precision:

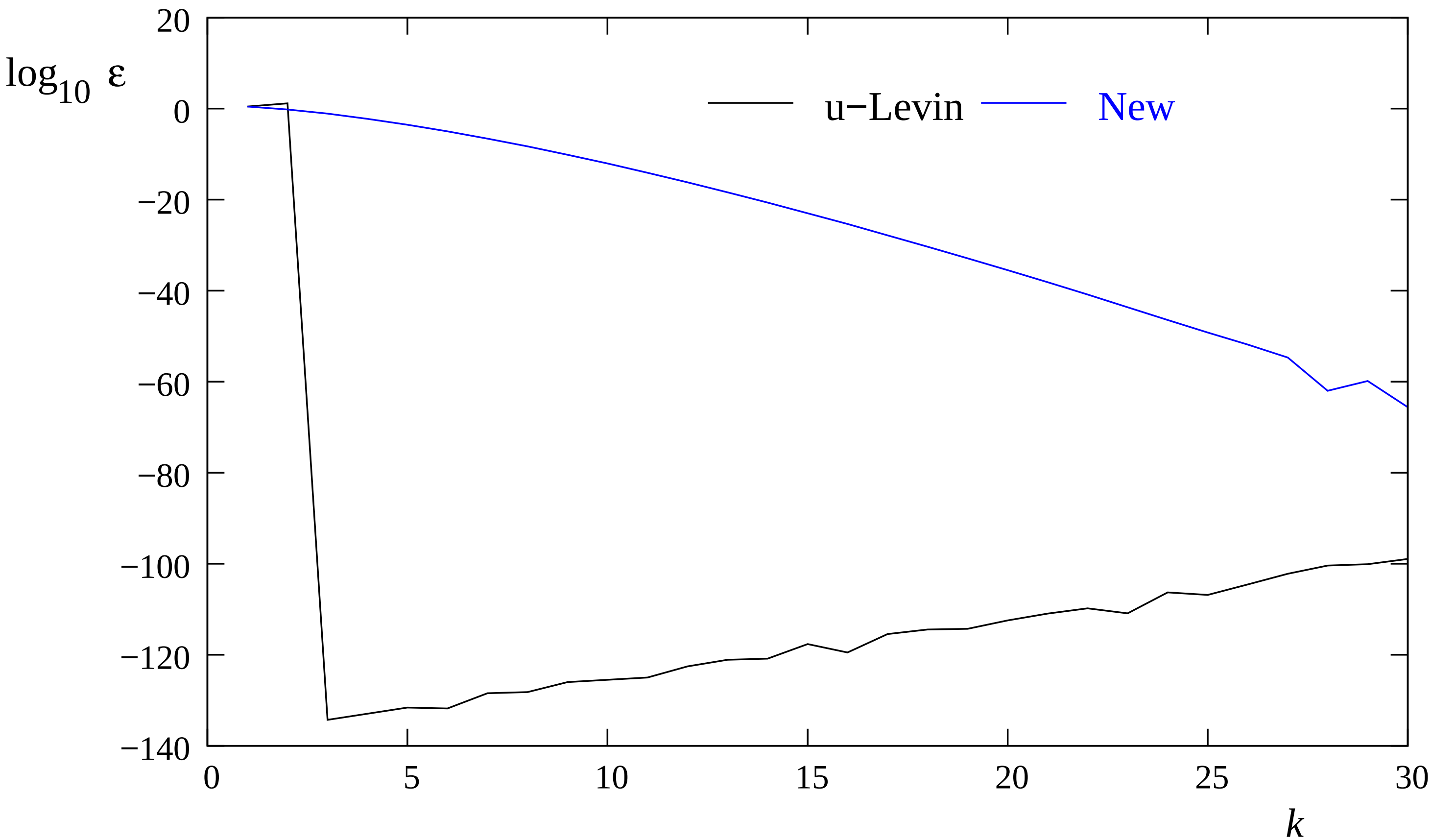
- MPFR: Multi-Precision Floating-point library with correct Rounding (free distribution, in C language).
- L. Fousse, G. Hanrot, V. Lefevre, P. Pélissier and P. Zimmermann, *ACM Transactions on Mathematical Software*, **33**, 13:1-13:15 (2007).
- We adjust the number of bits of precision by convenience.

Recall Test 2:

- $$ {}_2F_1(1,1,5/2,1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3 $$

Recall Test 2:

- $${}_2F_1(1,1,5/2,1) = \sum_{n=0}^{\infty} \frac{n!}{(5/2)_n} = 3$$
- Results for 200 bit-precision:



Few electron integrals in atomic calculations

- Two electron correlated integrals:

$$I_2(i,j,l,a,b) = \int\int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-ar_1-br_2}$$

Few electron integrals in atomic calculations

- Two electron correlated integrals:

$$I_2(i,j,l,a,b) = \int\int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-ar_1-br_2}$$

- Usual approach:

$$r_{12}^l = \sum_{m=0}^{\infty} R_{l,m}(r_1,r_2) P_m(cos\theta_{12})$$

and expansions of $R_{l,m}$ in terms of $r_< = \min\{r_1,r_2\}$ and $r_> = \max\{r_1,r_2\}$ (finite sum) or $r_1 r_2/(r_1+r_2)^2$ (infinite sum).

Few electron integrals in atomic calculations

- Two electron correlated integrals:

$$I_2(i,j,l,a,b) = \int\int d\vec{r}_1 d\vec{r}_2 r_1^i r_2^j r_{12}^l e^{-ar_1 - br_2}$$

- Usual approach:

$$r_{12}^l = \sum_{m=0}^{\infty} R_{l,m}(r_1,r_2) P_m(cos\theta_{12})$$

and expansions of $R_{l,m}$ in terms of $r_< = \min\{r_1, r_2\}$ and $r_> = \max\{r_1, r_2\}$ (finite sum) or $r_1 r_2/(r_1+r_2)^2$ (infinite sum).

- The slowest convergent resulting series happens when $l = -2$ (relativistic and lower bound calculations)

- Particular case:

$$
\begin{aligned}
I_2(-2,-1,-2,a,b) &= \frac{8\pi^2}{b}\left\{\frac{\pi^2}{3} - \left[\ln\left(1+\frac{a}{b}\right)\right]^2\right. \\
&+ \left.\mathrm{Li}_2\left(1-\frac{a}{b}\right) - \mathrm{Li}_2\left(\frac{b}{b+a}\right)\right\} \quad [1]
\end{aligned}
$$

- Particular case:

$$I_2(-2,-1,-2,a,b) = \frac{8\pi^2}{b}\left\{\frac{\pi^2}{3} - \left[\ln\left(1+\frac{a}{b}\right)\right]^2 + \mathrm{Li}_2\left(1-\frac{a}{b}\right) - \mathrm{Li}_2\left(\frac{b}{b+a}\right)\right\} \quad [1]$$

- Last two terms cancel some digits if $x = a/b$ is small.

- Particular case:

$$
\begin{aligned}
I_2(-2,-1,-2,a,b) &= \frac{8\pi^2}{b}\left\{\frac{\pi^2}{3} - \left[\ln\left(1+\frac{a}{b}\right)\right]^2\right. \\
&+ \left.\mathrm{Li}_2\left(1-\frac{a}{b}\right) - \mathrm{Li}_2\left(\frac{b}{b+a}\right)\right\} \quad [1]
\end{aligned}
$$

- Last two terms cancel some digits if $x = a/b$ is small.
-

$$
S(x) = \mathrm{Li}_2\left(1-x\right) - \mathrm{Li}_2\left(\frac{1}{1+x}\right) = \sum_{n=1}^{\infty}\frac{1}{n^2}\left[(1-x)^n - \left(\frac{1}{1+x}\right)^n\right]
$$

- Particular case:

$$I_2(-2,-1,-2,a,b) = \frac{8\pi^2}{b}\left\{\frac{\pi^2}{3} - \left[\ln\left(1+\frac{a}{b}\right)\right]^2 + \mathrm{Li}_2\left(1-\frac{a}{b}\right) - \mathrm{Li}_2\left(\frac{b}{b+a}\right)\right\} \quad [1]$$

- Last two terms cancel some digits if $x = a/b$ is small.
-

$$S(x) = \mathrm{Li}_2\left(1-x\right) - \mathrm{Li}_2\left(\frac{1}{1+x}\right) = \sum_{n=1}^{\infty}\frac{1}{n^2}\left[(1-x)^n - \left(\frac{1}{1+x}\right)^n\right]$$

- Very slowly convergent series if x is small (Rydberg states, Hydride ion).

- Particular case:

$$I_2(-2,-1,-2,a,b) = \frac{8\pi^2}{b}\left\{\frac{\pi^2}{3} - \left[\ln\left(1+\frac{a}{b}\right)\right]^2 + \mathrm{Li}_2\left(1-\frac{a}{b}\right) - \mathrm{Li}_2\left(\frac{b}{b+a}\right)\right\} \quad [1]$$

- Last two terms cancel some digits if $x = a/b$ is small.
-

$$S(x) = \mathrm{Li}_2\left(1-x\right) - \mathrm{Li}_2\left(\frac{1}{1+x}\right) = \sum_{n=1}^{\infty}\frac{1}{n^2}\left[(1-x)^n - \left(\frac{1}{1+x}\right)^n\right]$$

- Very slowly convergent series if x is small (Rydberg states, Hydride ion).

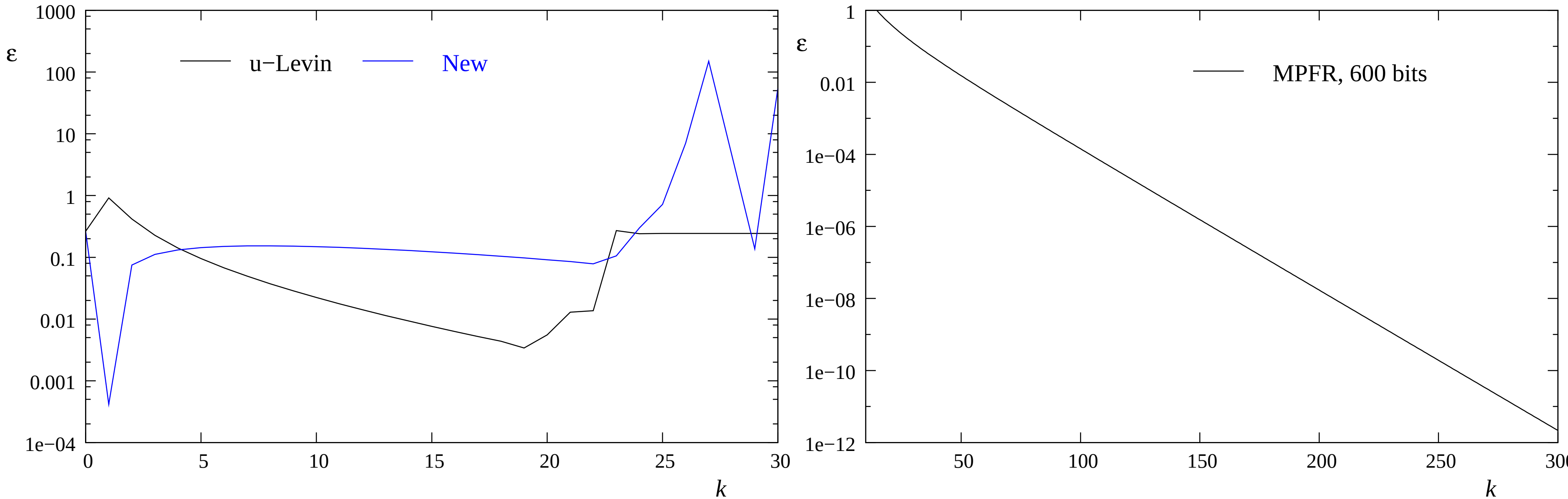
1 F.W. King, *Phys. Rev. A* **44**, 7108 (1991).

Test 5: $S(x = 0.001)$

- Use of $\alpha = 3/2$, although a_n does not behave as a negative power.

Test 5: $S(x = 0.001)$

- Use of $\alpha = 3/2$, although a_n does not behave as a negative power.
- $(n = 20)$



Three electron integrals

- $I_3(i,j,k,l,m,n,a,b,c) =$
$\int\int\int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1-br_2-cr_3}$

Three electron integrals

- $I_3(i,j,k,l,m,n,a,b,c) = \int\int\int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1-br_2-cr_3}$
- Multiple series when expanding r_{ij}, even more when avoiding $r_<$, $r_>$ (project with F.W. King and C. H. Leong).

Three electron integrals

- $I_3(i,j,k,l,m,n,a,b,c) = \int\int\int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1-br_2-cr_3}$
- Multiple series when expanding r_{ij}, even more when avoiding $r_<$, $r_>$ (project with F.W. King and C. H. Leong).
- Let us examine a particular case:

$$I_3(i,j,k,l,0,0,a,a,c) = \frac{(4\pi)^3}{\Gamma(-l/2)} \frac{(k+2)!}{c^{k+3}} \frac{(i+j+l+5)!}{a^{i+j+l+6}} S_l(i,j)$$

where

$$S_l(i,j) = \sum_{n=0}^{\infty} \frac{\Gamma(n-l/2)\Gamma(i+n+3)\Gamma(j+n+3)}{\Gamma(n+2)\Gamma(n+3+(i+j)/2)\Gamma(n+3+(i+j+1)/2)}$$

Three electron integrals

- $I_3(i,j,k,l,m,n,a,b,c) = \int\int\int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 r_1^i r_2^j r_3^k r_{12}^l r_{23}^m r_{31}^n e^{-ar_1-br_2-cr_3}$
- Multiple series when expanding r_{ij}, even more when avoiding $r_<$, $r_>$ (project with F.W. King and C. H. Leong).
- Let us examine a particular case:

$$I_3(i,j,k,l,0,0,a,a,c) = \frac{(4\pi)^3}{\Gamma(-l/2)} \frac{(k+2)!}{c^{k+3}} \frac{(i+j+l+5)!}{a^{i+j+l+6}} S_l(i,j)$$

where

$$S_l(i,j) = \sum_{n=0}^{\infty} \frac{\Gamma(n-l/2)\Gamma(i+n+3)\Gamma(j+n+3)}{\Gamma(n+2)\Gamma(n+3+(i+j)/2)\Gamma(n+3+(i+j+1)/2)}$$

- The general term behaves as $n^{-(l+5)/2}$. In practical variational calculations, the worst case is $l=-1$, for which $a_n \sim n^{-2}$.

- $S_{-1}(i,j)$ can be summed up exactly, and the remainder is known, for particular values of i and j.

- $S_{-1}(i, j)$ can be summed up exactly, and the remainder is known, for particular values of i and j.
- We will study the remainder for small values of i and j and trying to extrapolate the best accelerator.

- $S_{-1}(i,j)$ can be summed up exactly, and the remainder is known, for particular values of i and j.
- We will study the remainder for small values of i and j and trying to extrapolate the best accelerator.
- $S_{-1}(0,0)$:

$$S - S_n = (n+2)\, a_n \left[1 - \frac{5}{4(n+2)} - \frac{3}{8(n+2)^2}\right]$$
$$= n^{-1} \left[1 - \frac{9}{8(n+3/2)} - \frac{5}{8(n+5/2)}\right]$$

- $S_{-1}(i,j)$ can be summed up exactly, and the remainder is known, for particular values of i and j.
- We will study the remainder for small values of i and j and trying to extrapolate the best accelerator.
- $S_{-1}(0,0)$:

$$S - S_n = (n+2)\, a_n \left[1 - \frac{5}{4(n+2)} - \frac{3}{8(n+2)^2}\right]$$
$$= n^{-1} \left[1 - \frac{9}{8(n+3/2)} - \frac{5}{8(n+5/2)}\right]$$

- u-Levin exact for $\beta = 2$.

Other cases

- $S_{-1}(1,1)$:

$$S - S_n = (n+2)\,a_n \left[1 - \frac{13/8}{n+2} - \frac{13/8}{(n+2)^2} - \frac{5/8}{n+3}\right]$$

$$= n^{-1} \left[1 - \frac{15/16}{n+3/2} - \frac{3/8}{n+5/2} - \frac{7/16}{n+7/2}\right]$$

Other cases

- $S_{-1}(1,1)$:

$$\begin{aligned} S - S_n &= (n+2)\, a_n \left[1 - \frac{13/8}{n+2} - \frac{13/8}{(n+2)^2} - \frac{5/8}{n+3} \right] \\ &= n^{-1} \left[1 - \frac{15/16}{n+3/2} - \frac{3/8}{n+5/2} - \frac{7/16}{n+7/2} \right] \end{aligned}$$

- $S_{-1}(2,0)$:

$$\begin{aligned} S - S_n &= (n+2)\, a_n \left[1 - \frac{17/16}{n+2} - \frac{3/8}{(n+2)^2} - \frac{7/16}{n+4} \right] \\ &= n^{-1} \left[1 - \frac{21/16}{n+3/2} - \frac{5/8}{n+5/2} + \frac{7/16}{n+7/2} \right] \end{aligned}$$

Other cases

- $S_{-1}(1,1)$:

$$
\begin{aligned}
S - S_n &= (n+2)\, a_n \left[1 - \frac{13/8}{n+2} - \frac{13/8}{(n+2)^2} - \frac{5/8}{n+3}\right] \\
&= n^{-1} \left[1 - \frac{15/16}{n+3/2} - \frac{3/8}{n+5/2} - \frac{7/16}{n+7/2}\right]
\end{aligned}
$$

- $S_{-1}(2,0)$:

$$
\begin{aligned}
S - S_n &= (n+2)\, a_n \left[1 - \frac{17/16}{n+2} - \frac{3/8}{(n+2)^2} - \frac{7/16}{n+4}\right] \\
&= n^{-1} \left[1 - \frac{21/16}{n+3/2} - \frac{5/8}{n+5/2} + \frac{7/16}{n+7/2}\right]
\end{aligned}
$$

- $S_{-1}(2,2)$:

$$
\begin{aligned}
S - S_n &= (n+2)\, a_n \left[1 - \frac{477/256}{n+2} - \frac{45/128}{(n+2)^2} + \frac{45/64}{n+3} + \frac{105/256}{n+4}\right] \\
&= n^{-1} \left[1 - \frac{105/128}{n+3/2} - \frac{75/128}{n+5/2} - \frac{76/128}{n+7/2} - \frac{45/128}{n+9/2}\right]
\end{aligned}
$$

Weniger transformation

- For a series for which:

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)_j}$$

Weniger transformation

- For a series for which:

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)_j}$$

- Then, multiplying by $(n+\beta)_{k-1}$ both sides:

$$(n+\beta)_{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree} \quad k-1$$

Weniger transformation

- For a series for which:

$$S_n = S + \omega_n \sum_{j=0}^{k-1} \frac{C_j}{(n+\beta)_j}$$

- Then, multiplying by $(n+\beta)_{k-1}$ both sides:

$$(n+\beta)_{k-1} \frac{S_n - S}{\omega_n} = \text{polynomial in } n \text{ of degree } \quad k-1$$

- And applying Δ^k to this equation:

$$S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)_{k-1}}{(n+k+\beta)_{k-1}} \frac{S_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\beta)_{k-1}}{(n+k+\beta)_{k-1}} \frac{1}{\omega_{n+j}}}$$

Generalization

- For a series for which:

$$
\begin{aligned}
S_n &= S + \omega_n \left[C_0 + \frac{C_{11}}{n+\beta_1} + \frac{C_{12}}{(n+\beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n+\beta_1)^{p_1}} + \cdots \right. \\
&+ \left. \frac{C_{l1}}{n+\beta_l} + \frac{C_{l2}}{(n+\beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n+\beta_l)^{p_l}} + \cdots \right]
\end{aligned}
$$

Generalization

- For a series for which:

$$
\begin{aligned}
S_n \quad &= \quad S + \omega_n \left[C_0 + \frac{C_{11}}{n+\beta_1} + \frac{C_{12}}{(n+\beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n+\beta_1)^{p_1}} + \cdots \right. \\
&+ \quad \left. \frac{C_{l1}}{n+\beta_l} + \frac{C_{l2}}{(n+\beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n+\beta_l)^{p_l}} + \cdots \right]
\end{aligned}
$$

- Multiplying by $(n+\beta_1)^{p_1} \cdots (n+\beta_l)^{p_l}$ and applying Δ^k with $k = p_1 + p_2 + \cdots p_l + 1$

$$
S = \frac{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{S_{n+j}}{\omega_{n+j}}}{\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{1}{\omega_{n+j}}}
$$

where $\alpha_1 = \cdots \alpha_{p_1} = \beta_1$, $\alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2$, and so on.

Generalization

- For a series for which:

$$S_n = S + \omega_n \left[C_0 + \frac{C_{11}}{n+\beta_1} + \frac{C_{12}}{(n+\beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n+\beta_1)^{p_1}} + \cdots \right.$$
$$\left. + \frac{C_{l1}}{n+\beta_l} + \frac{C_{l2}}{(n+\beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n+\beta_l)^{p_l}} + \cdots \right]$$

- Multiplying by $(n+\beta_1)^{p_1}\cdots(n+\beta_l)^{p_l}$ and applying Δ^k with $k = p_1 + p_2 + \cdots p_l + 1$

$$S = \frac{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{S_{n+j}}{\omega_{n+j}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{1}{\omega_{n+j}}}$$

where $\alpha_1 = \cdots \alpha_{p_1} = \beta_1$, $\alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2$, and so on.

- This is a generalization (including ω_n) of the generalization of Levin and Weniger transform by Čížek-Zamastil-Skála, also studied by Weniger.

Generalization

- For a series for which:

$$S_n = S + \omega_n \left[C_0 + \frac{C_{11}}{n+\beta_1} + \frac{C_{12}}{(n+\beta_1)^2} + \cdots + \frac{C_{1p_1}}{(n+\beta_1)^{p_1}} + \cdots \right.$$
$$\left. + \frac{C_{l1}}{n+\beta_l} + \frac{C_{l2}}{(n+\beta_l)^2} + \cdots + \frac{C_{lp_l}}{(n+\beta_l)^{p_l}} + \cdots \right]$$

- Multiplying by $(n+\beta_1)^{p_1} \cdots (n+\beta_l)^{p_l}$ and applying Δ^k with $k = p_1 + p_2 + \cdots p_l + 1$

$$S = \frac{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{S_{n+j}}{\omega_{n+j}}}{\displaystyle\sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{(n+j+\alpha_1)\cdots(n+j+\alpha_k)}{(n+k+\alpha_1)\cdots(n+k+\alpha_k)} \frac{1}{\omega_{n+j}}}$$

where $\alpha_1 = \cdots \alpha_{p_1} = \beta_1$, $\alpha_{p_1+1} = \cdots \alpha_{p_1+p_2} = \beta_2$, and so on.

- This is a generalization (including ω_n) of the generalization of Levin and Weniger transform by Čížek-Zamastil-Skála, also studied by Weniger.

Application:

- For $S_{-1}(i, j)$ sums, previous formula can be applied:

Application:

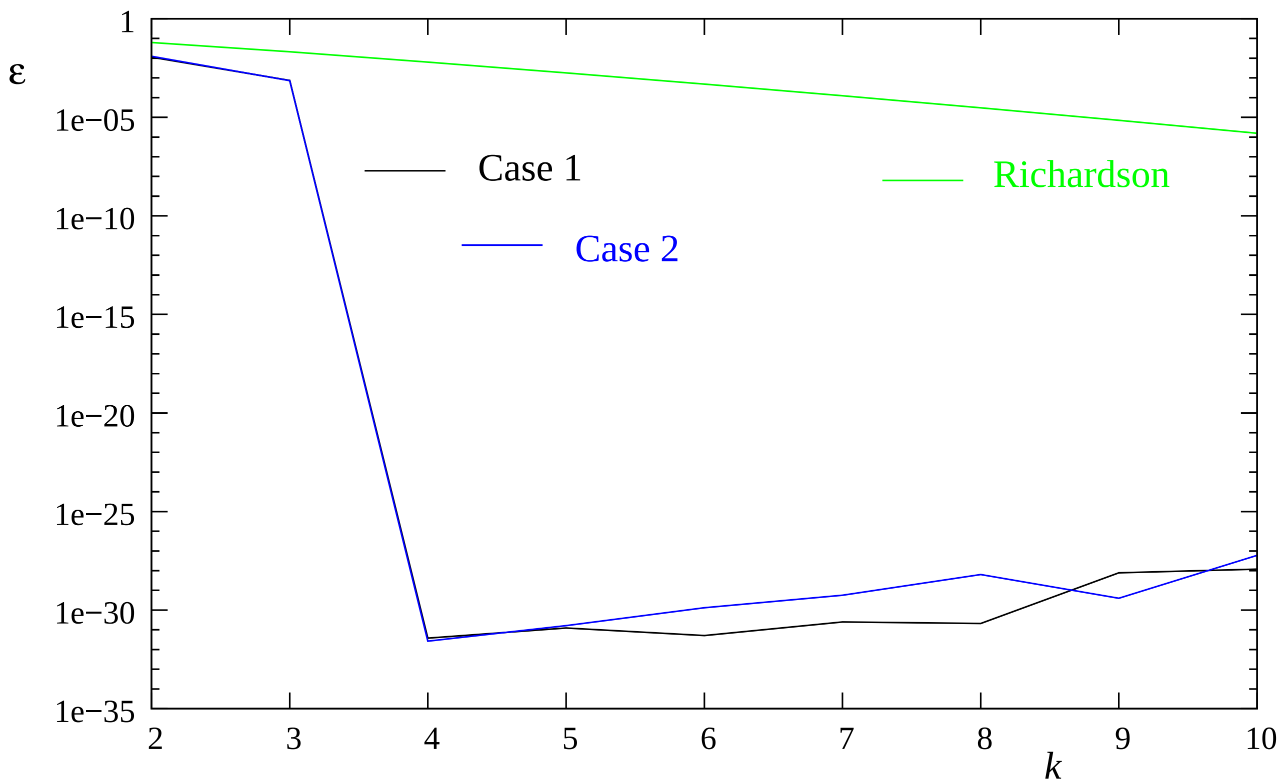
- For $S_{-1}(i,j)$ sums, previous formula can be applied:
- Case 1: Use $\omega_n = (n+2)a_n$ and $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = \alpha_4 = 3$, . . .

Application:

- For $S_{-1}(i,j)$ sums, previous formula can be applied:
- Case 1: Use $\omega_n = (n+2)a_n$ and $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = \alpha_4 = 3$, ...
- Case 2: Use $\omega_n = n^{-1}$ and $\alpha_i = i + 1/2$

Application:

- For $S_{-1}(i,j)$ sums, previous formula can be applied:
- Case 1: Use $\omega_n = (n+2)a_n$ and $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = \alpha_4 = 3$, ...
- Case 2: Use $\omega_n = n^{-1}$ and $\alpha_i = i + 1/2$
- $S_1(1,1)$:



Conclusions:

- $\omega_n = (n+\beta)^{-\alpha+1}$ is a interesting alternative to u-Levin when $a_n \sim n^{-\alpha}$

Conclusions:

- $\omega_n = (n+\beta)^{-\alpha+1}$ is a interesting alternative to u-Levin when $a_n \sim n^{-\alpha}$
- Use of differences of partial sums instead of S_{n+j} improves slightly the optimal result.

Conclusions:

- $\omega_n = (n+\beta)^{-\alpha+1}$ is a interesting alternative to u-Levin when $a_n \sim n^{-\alpha}$
- Use of differences of partial sums instead of S_{n+j} improves slightly the optimal result.
- Multiple precision calculations are required for some very slowly converging series.

Conclusions:

- $\omega_n = (n+\beta)^{-\alpha+1}$ is a interesting alternative to u-Levin when $a_n \sim n^{-\alpha}$
- Use of differences of partial sums instead of S_{n+j} improves slightly the optimal result.
- Multiple precision calculations are required for some very slowly converging series.
- Generalization of the transformation of Čížek et al. is adequate for the three-electron integral problem.

Conclusions:

- $\omega_n = (n+\beta)^{-\alpha+1}$ is a interesting alternative to u-Levin when $a_n \sim n^{-\alpha}$
- Use of differences of partial sums instead of S_{n+j} improves slightly the optimal result.
- Multiple precision calculations are required for some very slowly converging series.
- Generalization of the transformation of Čížek et al. is adequate for the three-electron integral problem.
- Weniger's treatment using Δ^k is a powerful formalism for the design of convergence accelerators.