Review of the collaboration between

Israel Koltracht (Mathemtics Dept., UCONN)
and
George Rawitscher (Physics Dept., UCONN)

IWOTA 2008, July 22 – 26, 2008

presented by G. Rawitscher

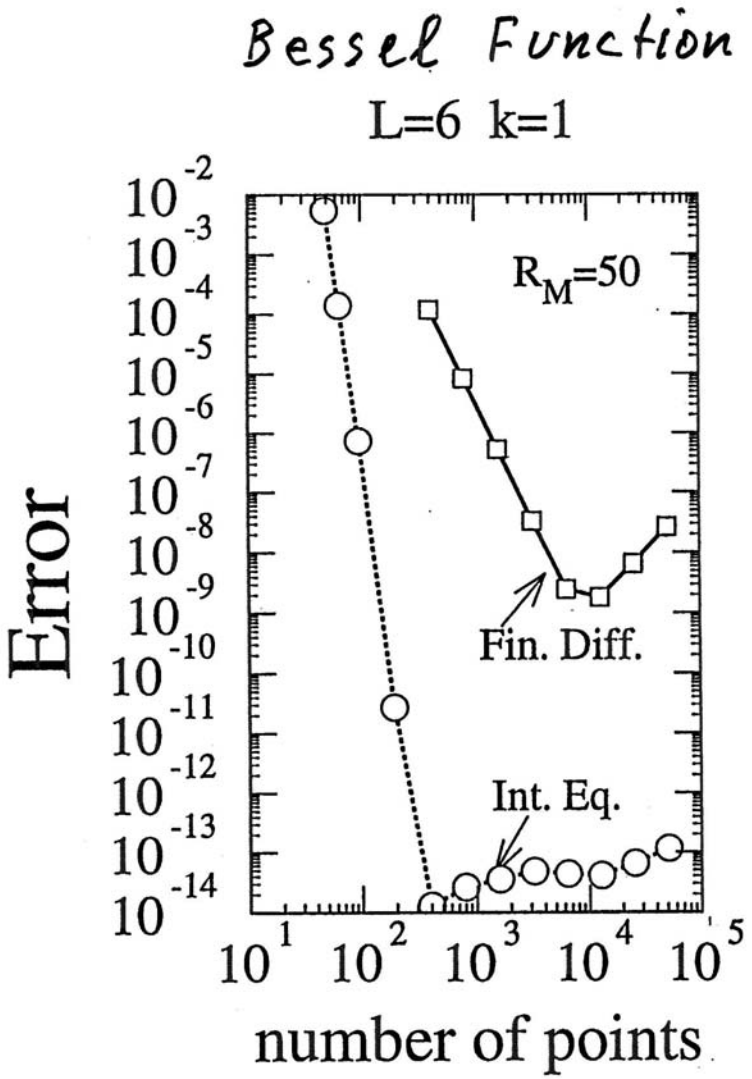
Integral Eq. method (IEM)

1. The solution of Integral Eq. is numerically more stable than the solution of Differential Eq.

2. The expansion of a function into Chebyshev Polynomials converges rapidly and the truncation errors are known;

3. Division of total interval into partitions permits a very efficient distribution of mesh-points.

So far this holds for the one-dimensional Schr. Eq. in config. space.



Gonzales
Eisert
Koltracht
Neumann
Rawitscher

J. Comp. Phys.
134 134 (1997)

Primer on Chebyshev Polynomials $\mathbf{T}_n(\mathbf{x}) = \cos(\mathbf{n\theta})$:

Expansion error:

If $f(x) \in C^p[-1,1]$ then

$$\left| f(x) - \sum_{k=0}^{N} a_k T_k(x) \right| \leq \frac{c}{p-1} \frac{1}{N^{p-1}}$$

If $f(x)$ is $\infty' ly$ differentiable then
the expansion converges faster than any power of N

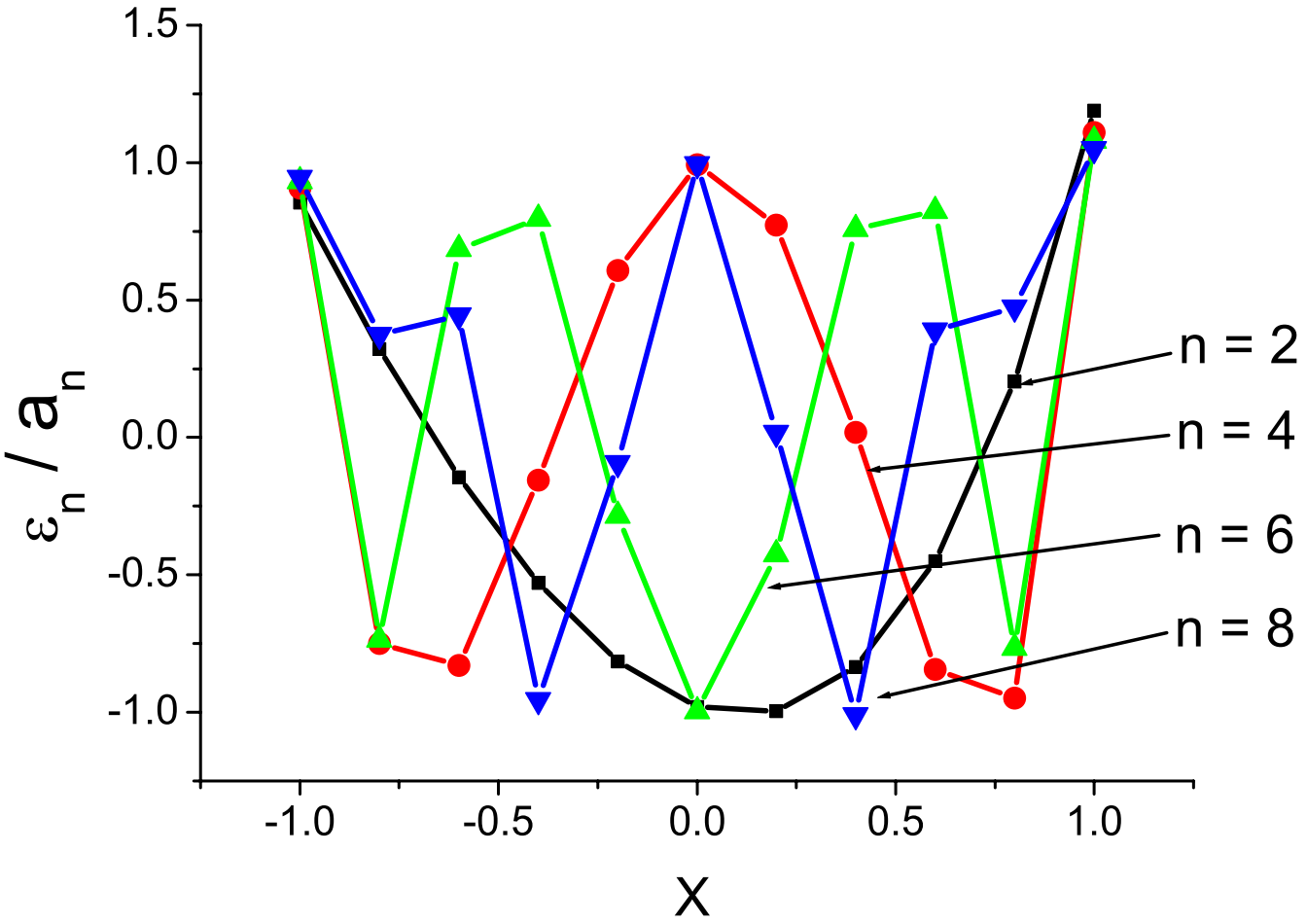
Example: $f(x) = e^{x}$

$[-1\ ,\ 1]$

$$a_k = \frac{2}{\pi} \int_{-1}^{1} e^{x}\ T_k(x)\ (1 - x^2)^{-1/2}\ dx$$

$$a_k = 2\, I_k(1) \simeq \frac{2}{\sqrt{2\pi\, k}} \left(\frac{e}{2\, k} \right)^{k}$$

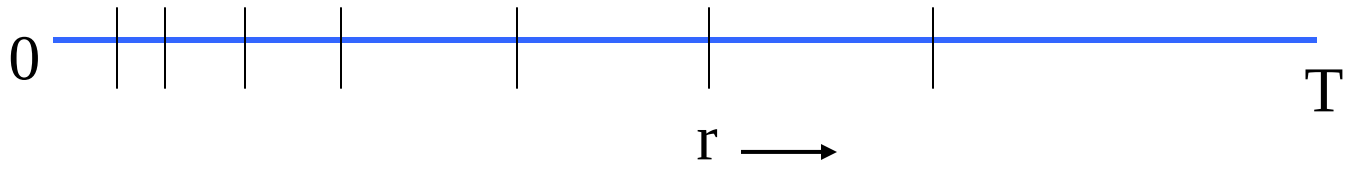
Modiied Bessel fctn


1.5
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0
X
ε_n / a_n
n = 2
n = 4
n = 6
n = 8

Method of solving Integral Eqs. (IEM)

$$(d^2/dr^2 + k^2)\psi = V\psi$$

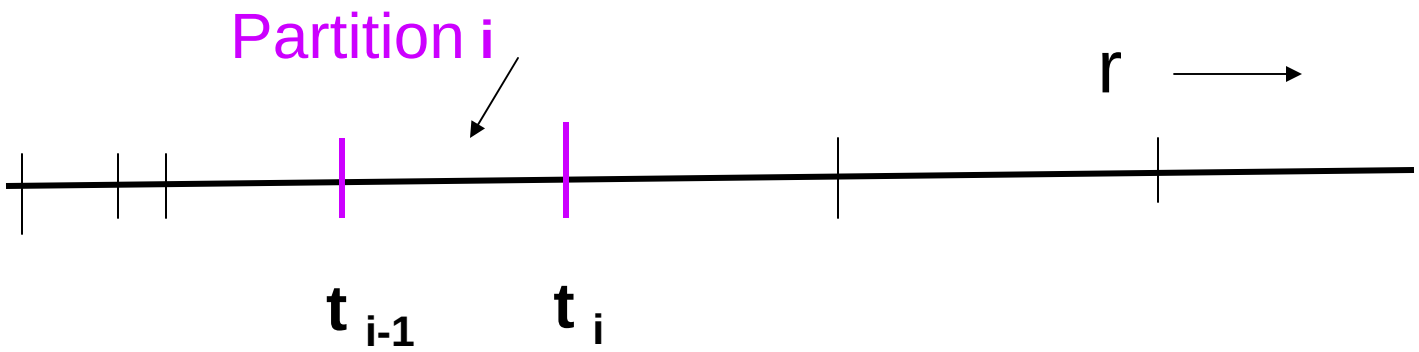
$$\psi(r) = \sin(kr) + \int_0^T \mathcal{G}_0(r,r')\,V(r')\,\psi(r')\,dr'$$



$$\mathcal{G}_0 = -(1/k)\,\sin(kr_<)\,\cos(kr_>)$$

Ψ(r) $\longrightarrow$ sin (kr + δ)

The Integral Eq. Algorithm



$$\psi(r) = A_i Y_i(r) + B_i Z_i(r), \quad t_{i-1} \le r \le t_i,$$

Calc. of the coefficients A and B

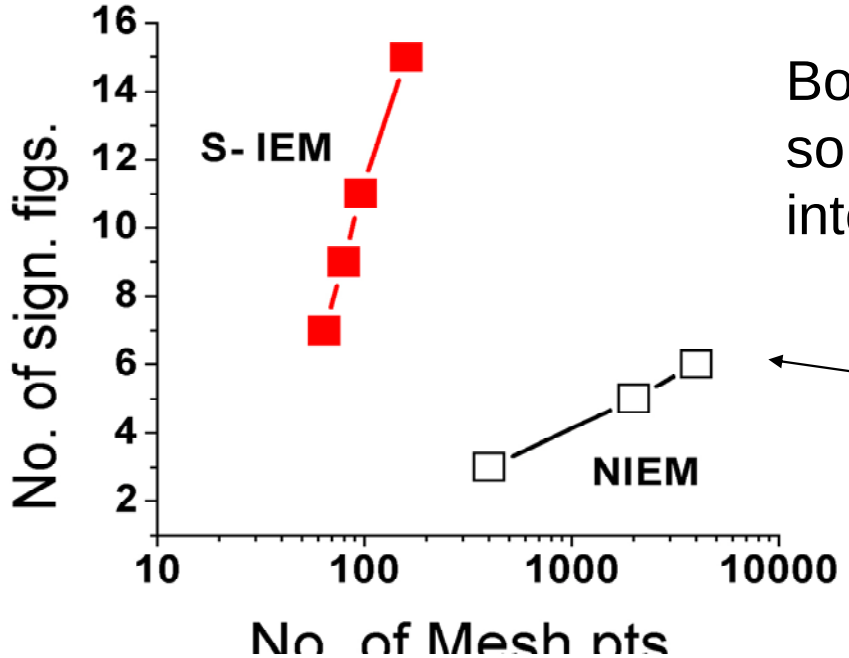
$$\begin{bmatrix} I & M_{12} & & 0 & 0 & 0 \\ M_{21} & I & M_{23} & 0 & 0 & 0 \\ & M_{32} & \ddots & & & \\ 0 & 0 & & \ddots & & \\ 0 & 0 & & & I & M_{m-1,m} \\ 0 & 0 & & & M_{m,m-1} & I \end{bmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \vdots \\ \alpha_{m-1} \\ \alpha_m \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ u \end{pmatrix}.$$

$$\alpha_j = \begin{pmatrix} A_j \\ B_j \end{pmatrix}; \qquad u = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \qquad 0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

8 papers with I. Koltracht from 1996 to 2006

Examples

e-H scattering with exchange; Error in the singlet phase-shift

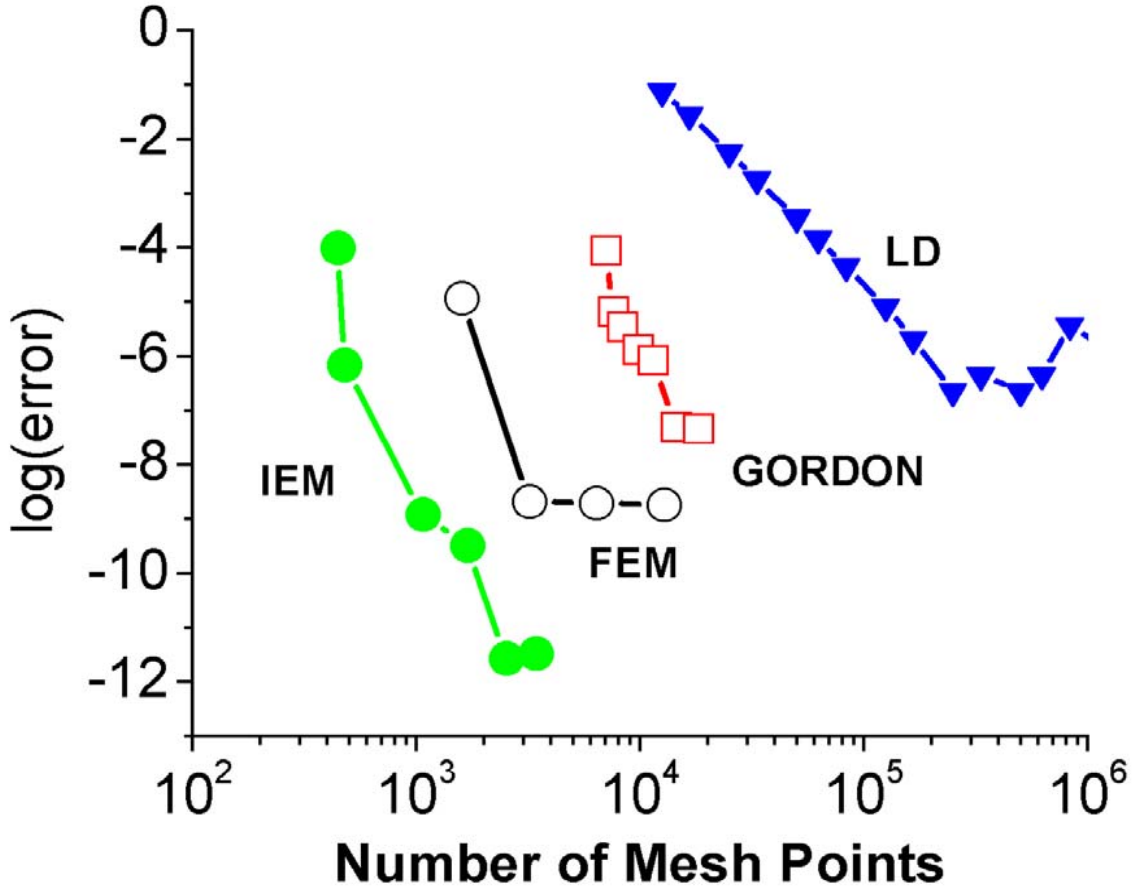


Both methods solve the same integral eqn.

Sams & Kouri
J. Ch. Phys (69)

Kang, Koltracht, Rawitscher, J. Chem. Phys., **118,** 9145 (2003)

Scattering of two atoms, including an open and a bound Channel



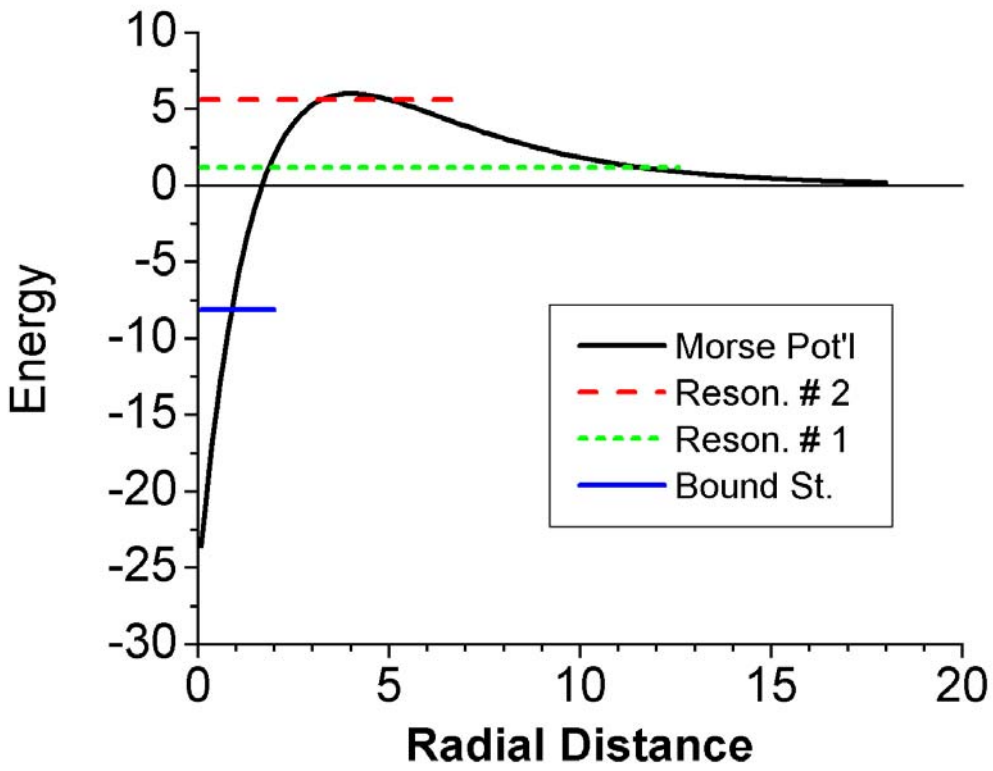
Rawitscher,
Esry, Tiesinga
Burke, Koltracht

J. Chem Phys.
111, 10418 (1999)

Barrier Penetration in a Morse Potential

$$V(r) = A\, e^{-(r-r_e)\alpha}\left(2 - e^{-(r-r_e)\alpha}\right)$$

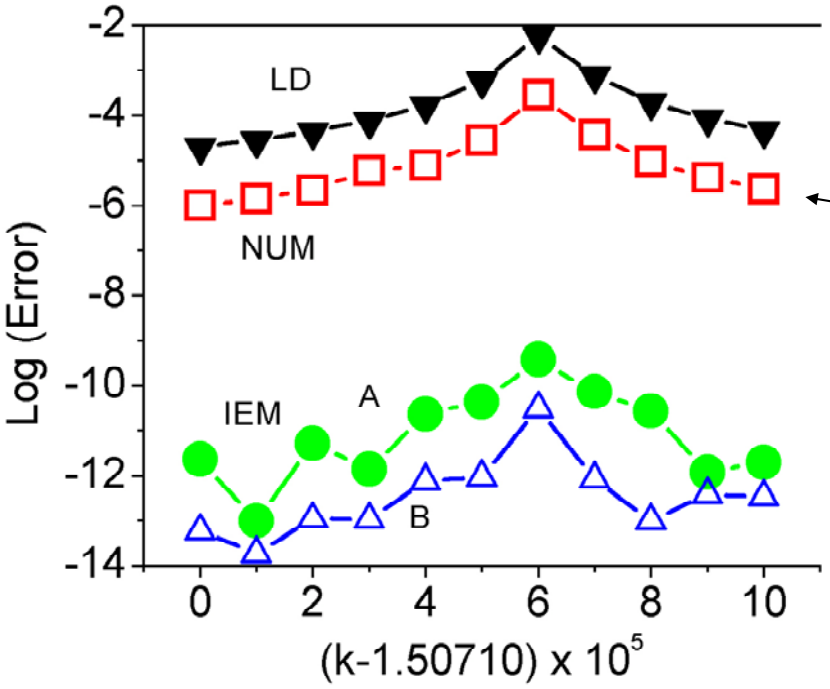
0< r < inf.



A = 6 fm $^{-2}$
r_e = 4 fm
a = 0.3 fm^{-1}

G. Rawitscher,
C. Merow,
M. Nguyen
I. Simbotin
Am. J. of Physics,
70, 935 (2002)

Error of the resonant phase shift in a Morse Pot'l



Molscat, Balakrishnan

Zerrad

Rawitscher & Koltracht
CiSE **7**, 58 (2005)

Calculation of the He-He binding energy

with an integral equation method.

Rawitscher and Koltracht, Eur. J. Phys **27**, 1179 (2006)

The bound-state integral equation

$$\psi(r) = \int_0^T \mathcal{G}(r,r')V(r')\psi(r')dr'$$

$$\mathcal{G}(r,r') = -\frac{1}{\kappa}F(r_<)G(r'_>)$$

$$F(r) = \sinh(\kappa r), \qquad G(r) = \exp(-\kappa r)$$

Iterate

$$\kappa_{s+1} = \kappa_s - (Iter)_s$$

Propagation from one partition to the next

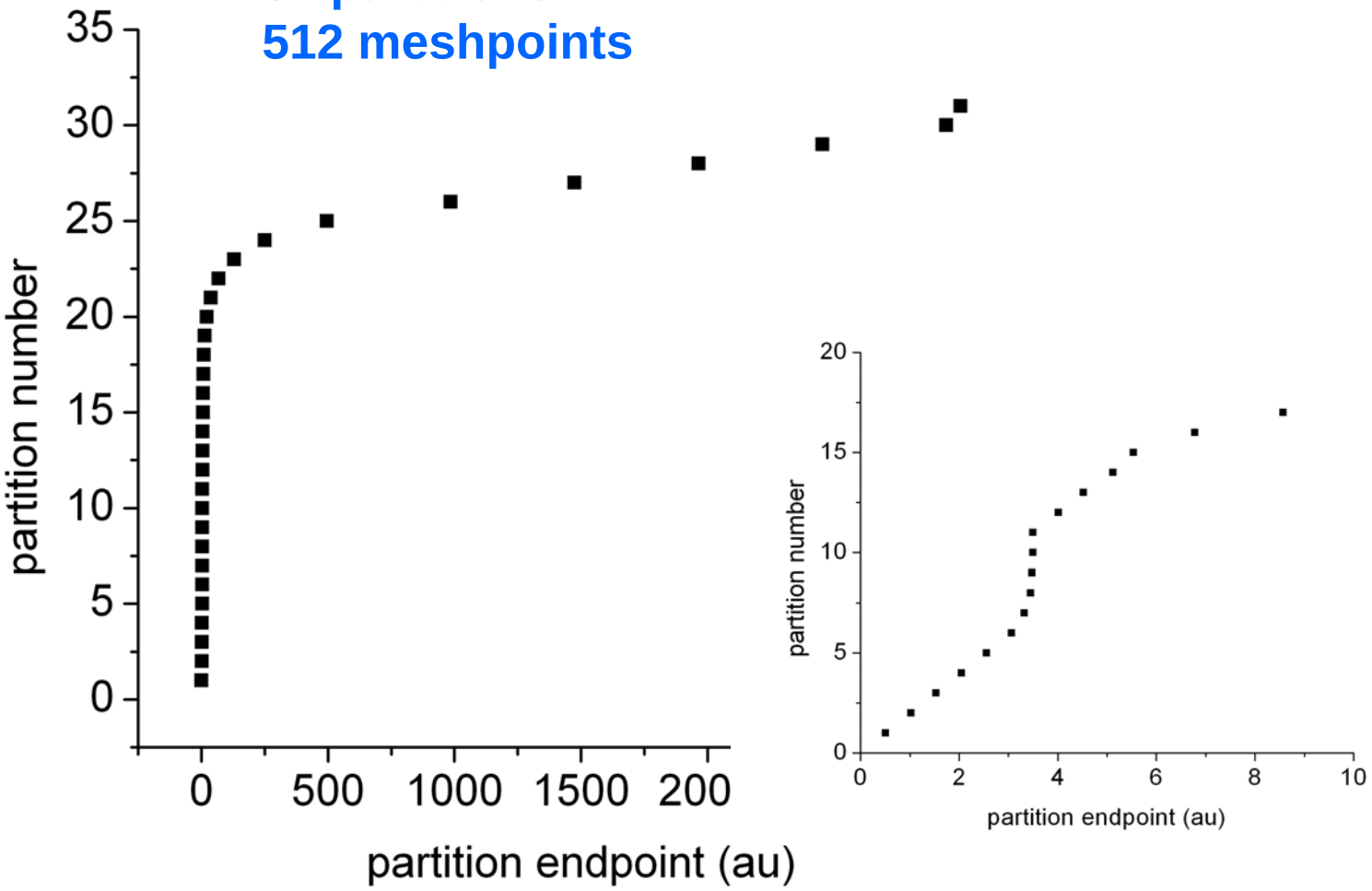
$$E_i = \exp(-\kappa t_i) \qquad \psi(r) = a_i y_i(r) + b_i z_i(r)$$

$$\begin{pmatrix} E_i/E_{i+1} & 0 \\ 0 & E_{i+1}/E_i \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1-(gy)_{i+1} & -(gz)_{i+1} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}_{i+1}$$

$$= \begin{pmatrix} -(fy)_i & 1-(fz)_i \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}_i$$

He-He Partition distribution, IEM

32 partitions
512 meshpoints



Result: We converge to the He-He diatom binding Energy to better than 8 significant figs.

Next? Solution of the quantum three-body problem in configuration space

Conclusion: We all miss Israel Koltracht