TAYLOR SERIES METHOD FOR SYSTEM OF PARTICLES INTERACTING VIA LENNARD-JONES POTENTIAL

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Mathematical model

We consider the Hamiltonian :

$$\boldsymbol{H(p,q)} = \frac{1}{2}\sum_{i=1}^{N}\frac{1}{m}\boldsymbol{p_i^T p_i} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} 4\varepsilon[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}]$$

$\boldsymbol{r_{ij}} = \|\boldsymbol{q_i} - \boldsymbol{q_j}\|_2$ is the distance between i-th and j-th particles.
$\boldsymbol{m, \varepsilon, \sigma}$ are suitable constants depending on the atoms.
We normalize time and space this way:

$$\tilde{t} = \frac{t}{\sigma m^{1/2}\varepsilon^{-1/2}}, \tilde{q} = \frac{q}{\sigma}$$

Omitting tilde we have the normalized system:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = 24\sum_{j=1}^{N}(2(\frac{1}{r_{ij}})^{14} - (\frac{1}{r_{ij}})^{8})(q_i - q_j)$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = p_i$$

$\boldsymbol{p_i}$ and $\boldsymbol{q_i}$ are vectors in $\boldsymbol{R^d, d = 1, 2, 3}$ but we omit the arrow $\longrightarrow$.
The only exception is next slide.

Numerical method - Taylor Series Method

We need to calculate derivatives (with respect to time) of solution via partial derivatives of H. For example for second derivatives we have

$$\frac{d^2\vec{q}_i(t)}{dt^2} = \sum_{j=1}^{N}\left[-\frac{\partial^2 H}{\partial\vec{p}_i\partial\vec{p}_j}\frac{\partial H}{\partial\vec{q}_j} + \frac{\partial^2 H}{\partial\vec{p}_i\partial\vec{q}_j}\frac{\partial H}{\partial\vec{p}_j}\right], \qquad i = 1,\ldots,N.$$

$$\frac{d^2\vec{p}_i(t)}{dt^2} = \sum_{j=1}^{N}\left[\frac{\partial^2 H}{\partial\vec{q}_i\partial\vec{p}_j}\frac{\partial H}{\partial\vec{q}_j} - \frac{\partial^2 H}{\partial\vec{q}_i\partial\vec{q}_j}\frac{\partial H}{\partial\vec{p}_j}\right], \qquad i = 1,\ldots,N.$$

Let $\overrightarrow{r} = (\overrightarrow{q_1}, \overrightarrow{q_2}, \ldots\overrightarrow{q_N}, \overrightarrow{p_1}, \overrightarrow{p_2}, \ldots, \overrightarrow{p_N})^T$

Explicit Taylor method

$$\vec{r}(t+\Delta t) = \sum_{j=0}^{n}\frac{\vec{r}^{(j)}(t)(\Delta t)^j}{j!}$$

Implicit Taylor method

$$\vec{r}(t) = \sum_{j=0}^{n}\frac{\vec{r}^{(j)}(t+\Delta t)(-\Delta t)^j}{j!},$$

For second derivatives in our case we have:

$$\ddot{\boldsymbol{q}}_i = \dot{\boldsymbol{p}}_i = 24\sum_{j=1}^{N}(2(\frac{1}{\boldsymbol{r}_{ij}})^{14} - (\frac{1}{\boldsymbol{r}_{ij}})^{8})(\boldsymbol{q}_i - \boldsymbol{q}_j)$$

$$\ddot{\boldsymbol{p}}_i = 24\sum_{j=1}^{N}(-28(\frac{1}{\boldsymbol{r}_{ij}})^{16}+8(\frac{1}{\boldsymbol{r}_{ij}})^{10})((\boldsymbol{q}_i - \boldsymbol{q}_j)^T(\boldsymbol{p}_i-\boldsymbol{p}_j))(\boldsymbol{q}_i-\boldsymbol{q}_j)$$

$$+24\sum_{j=1}^{N}(2(\frac{1}{\boldsymbol{r}_{ij}})^{14} - (\frac{1}{\boldsymbol{r}_{ij}})^{8})(\boldsymbol{p}_i - \boldsymbol{p}_j)$$

Third derivatives are also easy to calculate but they have more sums. We use them in our calculations.

We denote explicit method that use first derivative with $\boldsymbol{ex1}$.
This is actually **Explicit Euler** method.
Implicit method that use fist derivative is $\boldsymbol{im1}$.
This is actually **Implicit Euler**.
The methods that use first and second derivatives are $\boldsymbol{ex2}$ and $\boldsymbol{im2}$.
The methods that use first,second and third derivatives
are $\boldsymbol{ex3}$ and $\boldsymbol{im3}$.
We also consider composition methods (half step with implicit (explicit) and then half step explicit (implicit)).
We have in addition $\boldsymbol{ex1} \circ \boldsymbol{im1}$,$\boldsymbol{im1} \circ \boldsymbol{ex1}$, $\boldsymbol{ex2} \circ \boldsymbol{im2}$, $\boldsymbol{im2} \circ \boldsymbol{ex2}$,$\boldsymbol{ex3} \circ \boldsymbol{im3}$,$\boldsymbol{im3} \circ \boldsymbol{ex3}$.

Let us mention that:

- $\boldsymbol{ex1} \circ \boldsymbol{im1}$=**implicit midpoint rule** (symplectic)
- $\boldsymbol{im1} \circ \boldsymbol{ex1}$=**trapezidual rule**(not symplectic but also very good)
- **Verlet method** = one Seidel correction for $\boldsymbol{im1} \circ \boldsymbol{ex1}$

with explicit Euler with entire step as predictor.
Seidel correction means using already updated $\boldsymbol{q}$ for updating $\boldsymbol{p}$.

Predictor-corrector scheme

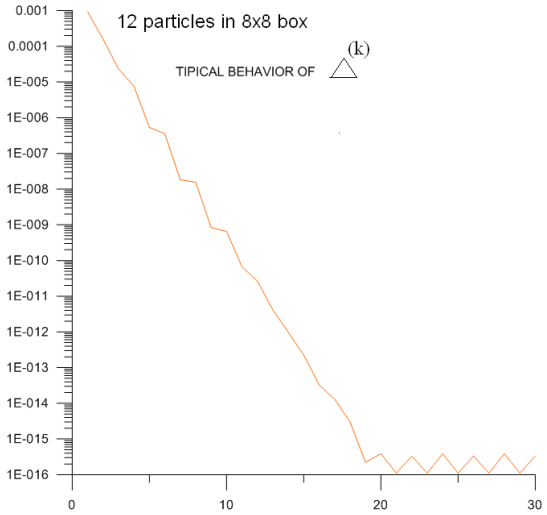
We solve implicit method as predictor-corrector. Predictor is the explicit formula of the same order. Corrections are with implicit formula. For example for $\boldsymbol{im2}$ we have.
Predictor:
$\boldsymbol{r^{(0)}(t+\tau) = r(t) + \tau\dot{r}(t) + \frac{\tau^2}{2}\ddot{r}(t)}$
Corrections:
$\boldsymbol{r^{(k+1)}(t+\tau) = r(t) + \tau\dot{r}(t+\tau)^{(k)} - \frac{\tau^2}{2}\ddot{r}(t+\tau)^{(k)}}$
This is simple iteration.

The derivatives of $\boldsymbol{p}$ depends on $\boldsymbol{q}$ and we can use already updated $\boldsymbol{q}$. This gives Seidel iteration which is actually better.

Stopping criterion for iterative process

Let $\Delta^{(k)} = \max\limits_{i=1,\ldots,N} \| \overrightarrow{r}_i^{(k)} - \overrightarrow{r}_i^{(k-1)} \|_\infty$
is the increment of two successive approximations.
N is the number of particles. $\overrightarrow{r_i} = (\overrightarrow{p_i}, \overrightarrow{q_i})$

Following Ernst Hairer we iterate until
either $\Delta^{(k)} = 0$ or $\Delta^{(k)} \geq \Delta^{(k-1)}$ which indicates that increments of the iteration start to oscillate due to roundoff.



Discretization error

Method	Leading term in local DE	Order of accuracy
ex1	$\frac{\tau u''}{2}$	1
im1	$-\frac{\tau u''}{2}$	1
im1$\bigcirc$ex1	$-\frac{\tau^2 u'''}{12}$	2
ex1$\bigcirc$im1	$\frac{\tau^2 u'''}{24}$	2

Discretization error

Method	Leading term in local DE	Order of accuracy
ex2	$\frac{\tau^2 u'''}{6}$	2
im2	$\frac{\tau^2 u'''}{6}$	2
im2$\bigcirc$ex2	$\frac{\tau^2 u'''}{24}$	2
ex2$\bigcirc$im2	$\frac{\tau^2 u'''}{24}$	2

Discretization error

Method	Leading term in local DE	Order of accuracy
ex3	$\frac{\tau^3 u''''}{24}$	3
im3	$-\frac{\tau^3 u''''}{24}$	3
im3$\bigcirc$ex3	$-\frac{\tau^4 u^{v}}{480}$	4
ex3$\bigcirc$im3	$\frac{\tau^4 u^{v}}{1920}$	4

Stability on the test equation of linear oscillator

We have the Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2, \omega > 0$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -\omega^2 q$$

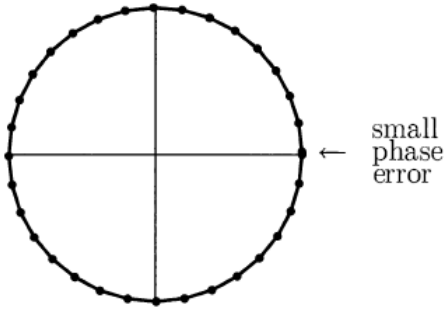
$$\dot{q} = \frac{\partial H}{\partial p} = p$$

Exact solution of the test initial problem is

$$\begin{pmatrix} p(t) \\ \omega q(t) \end{pmatrix} = \begin{pmatrix} \cos \omega t & -\sin \omega t \\ \sin \omega t & \cos \omega t \end{pmatrix} \begin{pmatrix} p(0) \\ \omega q(0) \end{pmatrix}$$

As we expect growth matrices for different methods are with truncated **cos** and **sin** series elements!

All composition methods give orthogonal matrices!
That means exactly conserving the energy for harmonic oscillator!
Remember that composition methods are
$ex1 \circ im1, im1 \circ ex1, ex2 \circ im2, im2 \circ ex2$
$ex3 \circ im3, im3 \circ ex3.$
For all of them we stay on the circle with small phase error of corresponding order of the method!



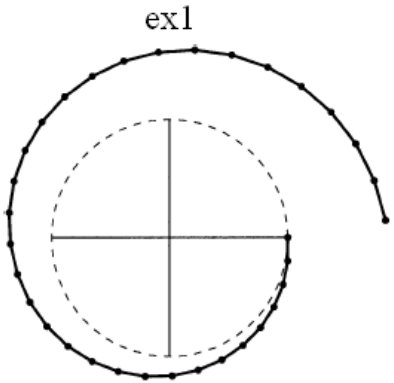
For example the growth matrix A for $ex1 \circ im1$ is:

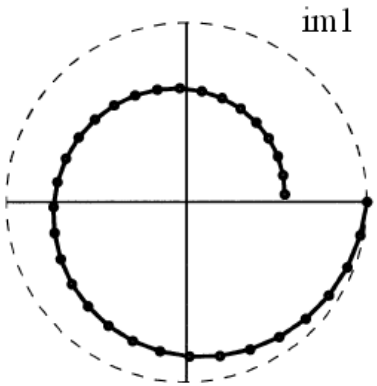
$$A = \begin{pmatrix} 1 & \frac{\tau\omega}{2} \\ -\frac{\tau\omega}{2} & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & -\frac{\tau\omega}{2} \\ \frac{\tau\omega}{2} & 1 \end{pmatrix}$$

Stability on the test equation of linear oscillator

Ex1 and ex2 are not stable for every choice of step τ!
The energy grows!

Im1 and im2 are stable for every choice of step τ!
But the energy decrease which is not physical!

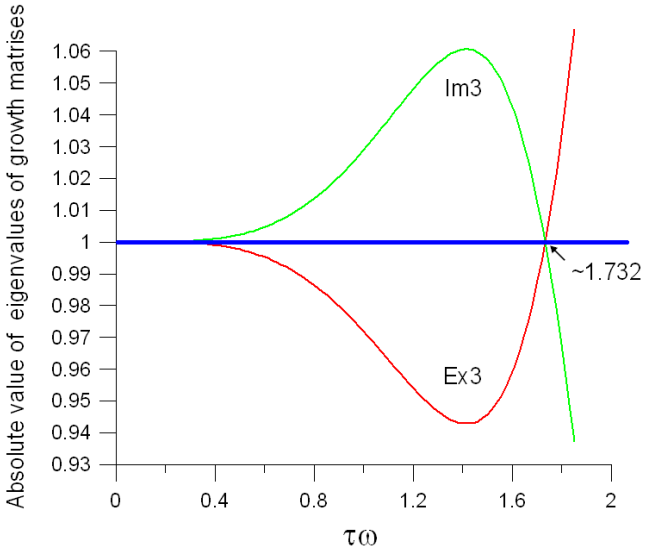




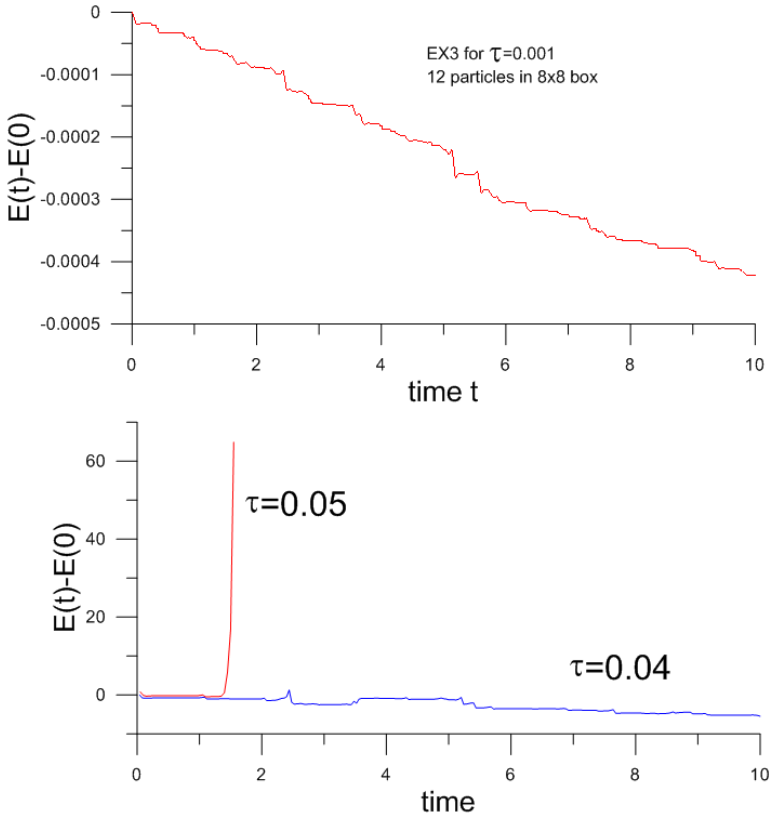
Stability on the test equation of linear oscillator

In contrast to Ex1 and Ex2, Ex3 is stable for certain step sizes.
As calculations show ex3 method is conditionally stable: $\tau\omega < 1.732$

In some cases Ex3 could be a good choice of method.



The experiments confirm the conditionally stability of Ex3.



Numerical experiments and results

We solve numerically two problems for our experiments.

1) Molecular analog of pendulum (two particles oscillator)

2) 12 particles in 8x8 box and periodic boundary conditions (as the example from the book of Gould and Tabochnik "An itroduction to computer simulation methods").

The experiments show that all composition methods behaves as symplectic, that is
The error in H is $\boldsymbol{O(\tau^k)}$.
The global error error is $\boldsymbol{O(t\tau^k)}$, $\boldsymbol{k}$ is the order of accuracy.

Simple iteration versus Seidel

Ex1○Im1 Simple Iterations, 12 particles in 8x8 box

step size	AVG ITER	MIN ITER	MAX ITER	Max|E(t)-E(0)| t∈[0,10]
0.01	14.57	9	27	0.63E-01
0.001	7.51	5	11	0.58E-03
0.0001	4.83	4	7	0.64E-05
0.00001	3.71	3	5	0.13E-06

Ex1○Im1 Seidel Iterations, 12 particles in 8x8 box

step size	AVG ITER	MIN ITER	MAX ITER	Max|E(t)-E(0)| t∈[0,10]
0.01	7.62	5	13	0.63E-01
0.001	4.10	3	6	0.58E-03
0.0001	3.00	2	4	0.64E-05
0.00001	2.08	2	3	0.13E-06

Simple iteration versus Seidel

Im3○Ex3 Simple iterations, 12 particles in 8x8 box

step size	AVG ITER	MIN ITER	MAX ITER	Max|E(t)-E(0)| t∈[0,10]
0.02	18.22	8	48	0.44E-02
0.01	12.53	6	21	0.46E-03
0.001	5.09	3	9	0.67E-05

Im3○Ex3 Seidel iterations, 12 particles in 8x8 box

step size	AVG ITER	MIN ITER	MAX ITER	Max|E(t)-E(0)| t∈[0,10]
0.02	10.12	6	18	0.44E-02
0.01	7.84	5	12	0.46E-03
0.001	4.47	3	6	0.67E-05

Testing for accuracy of $Im3 \circ Ex3$
Confirming fourth order accuracy

Im3○Ex3, 12 particles

Runge exponent $\alpha(t)$ for energy E(t)

$\alpha(t)=\log((E\tau(t)-E(0))/(E\tau/2(t)-E(0)))/\log(2)$

t	$\alpha(t)$	t	$\alpha(t)$	t	$\alpha(t)$	t	$\alpha(t)$
0.001	4.007	0.026	4.000	0.051	4.002	0.076	4.000
0.002	4.004	0.027	4.000	0.052	4.005	0.077	4.000
0.003	4.000	0.028	4.000	0.053	4.026	0.078	4.000
0.004	4.000	0.029	4.000	0.054	3.990	0.079	4.000
0.005	4.000	0.030	4.000	0.055	3.996	0.080	4.000
0.006	4.001	0.031	4.000	0.056	3.997	0.081	4.000
0.007	4.000	0.032	4.000	0.057	3.998	0.082	4.000
0.008	4.000	0.033	4.000	0.058	3.998	0.083	4.000
0.009	4.000	0.034	4.000	0.059	3.999	0.084	4.000
0.010	4.000	0.035	4.000	0.060	3.999	0.085	4.000
0.011	4.000	0.036	4.000	0.061	3.999	0.086	4.000
0.012	4.000	0.037	4.000	0.062	3.999	0.087	4.000
0.013	4.000	0.038	4.000	0.063	3.999	0.088	4.000
0.014	4.000	0.039	4.000	0.064	3.999	0.089	4.000
0.015	4.000	0.040	4.000	0.065	3.999	0.090	4.000
0.016	4.000	0.041	4.000	0.066	3.999	0.091	4.000
0.017	4.000	0.042	4.000	0.067	3.999	0.092	4.000
0.018	4.000	0.043	4.000	0.068	3.999	0.093	4.000
0.019	4.000	0.044	4.000	0.069	4.000	0.094	4.000
0.020	4.000	0.045	4.000	0.070	4.000	0.095	4.000
0.021	4.000	0.046	4.001	0.071	4.000	0.096	4.000
0.022	4.000	0.047	4.001	0.072	4.000	0.097	4.000
0.023	4.000	0.048	4.001	0.073	4.000	0.098	4.000
0.024	4.000	0.049	4.001	0.074	4.000	0.099	4.000
0.025	4.000	0.050	4.002	0.075	4.000	0.100	4.000

Testing for accuracy of $Im3 \circ Ex3$

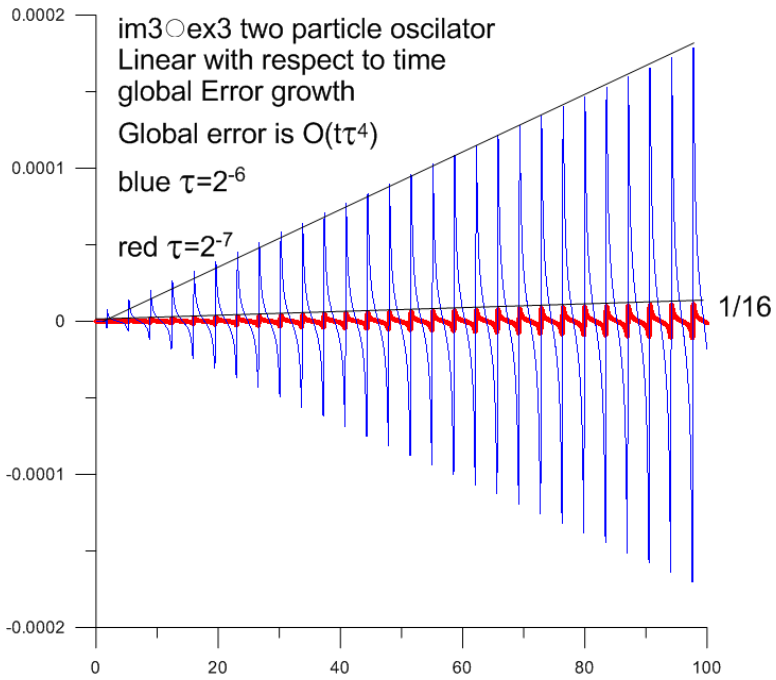
Im3○Ex3, 12 particles

Runge exponent $\alpha(t)$ for x-position x(t)
of a particular particle

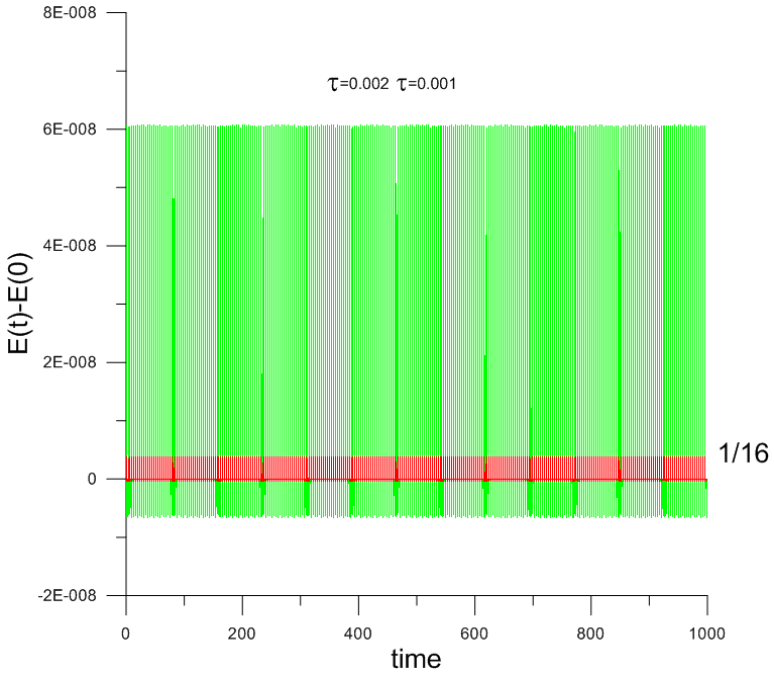
$\alpha(t)=\log((x\tau(t)-x\tau/2(t))/(x\tau/2(t)-x\tau/4(t)))/\log(2)$

t	$\alpha(t)$	t	$\alpha(t)$	t	$\alpha(t)$	t	$\alpha(t)$
0.001	4.002	0.026	4.000	0.051	4.000	0.076	4.000
0.002	4.003	0.027	4.000	0.052	4.000	0.077	4.000
0.003	4.002	0.028	4.000	0.053	4.000	0.078	4.000
0.004	4.002	0.029	4.000	0.054	4.000	0.079	4.000
0.005	4.001	0.030	4.000	0.055	4.000	0.080	4.000
0.006	4.001	0.031	4.000	0.056	4.000	0.081	4.000
0.007	4.000	0.032	4.000	0.057	4.000	0.082	4.000
0.008	4.000	0.033	4.000	0.058	4.000	0.083	4.000
0.009	4.000	0.034	4.000	0.059	4.000	0.084	4.000
0.010	4.000	0.035	4.000	0.060	4.000	0.085	4.000
0.011	4.000	0.036	4.000	0.061	4.000	0.086	4.000
0.012	4.000	0.037	4.000	0.062	4.000	0.087	4.000
0.013	4.000	0.038	3.999	0.063	4.000	0.088	4.000
0.014	4.000	0.039	3.999	0.064	4.000	0.089	4.000
0.015	4.000	0.040	3.997	0.065	4.000	0.090	4.000
0.016	4.000	0.041	4.002	0.066	4.000	0.091	4.000
0.017	4.000	0.042	4.000	0.067	4.000	0.092	4.000
0.018	4.000	0.043	4.000	0.068	4.000	0.093	4.000
0.019	4.000	0.044	4.000	0.069	4.000	0.094	4.000
0.020	4.000	0.045	4.000	0.070	4.000	0.095	4.000
0.021	4.000	0.046	4.000	0.071	4.000	0.096	4.000
0.022	4.000	0.047	4.000	0.072	4.000	0.097	4.000
0.023	4.000	0.048	4.000	0.073	4.000	0.098	4.000
0.024	4.000	0.049	4.000	0.074	4.000	0.099	4.000
0.025	4.000	0.050	4.000	0.075	4.000	0.100	4.000

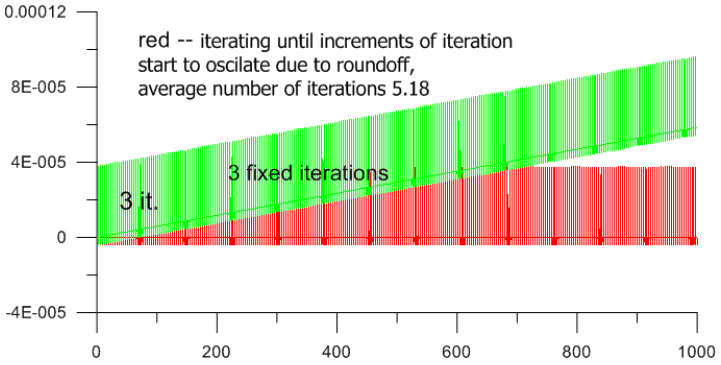
Global error behavior for molecule oscillator, $Im3 \circ Ex3$

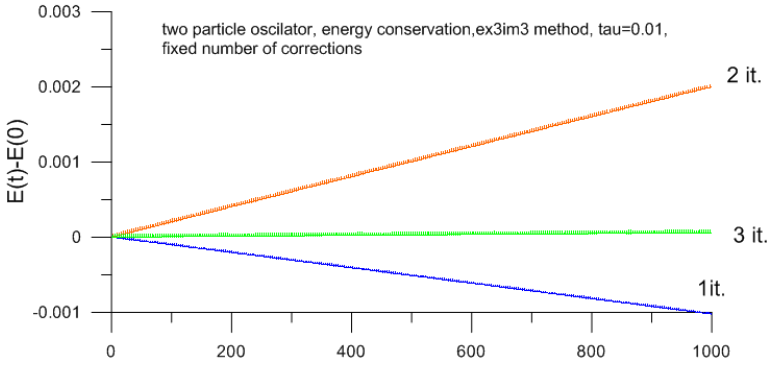


Long time integration for molecule oscillator, $Im3 \circ Ex3$



Long time integration for molecule oscillator, $Im3 \circ Ex3$





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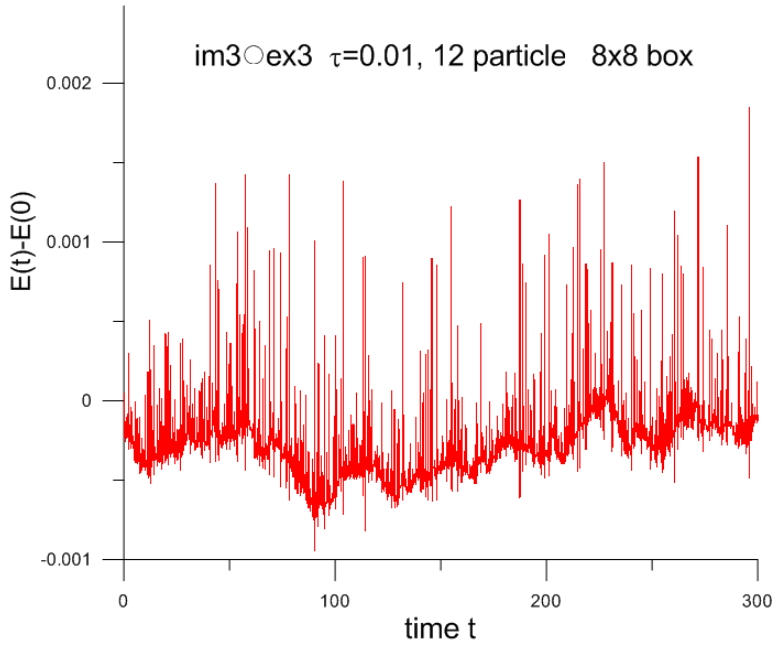
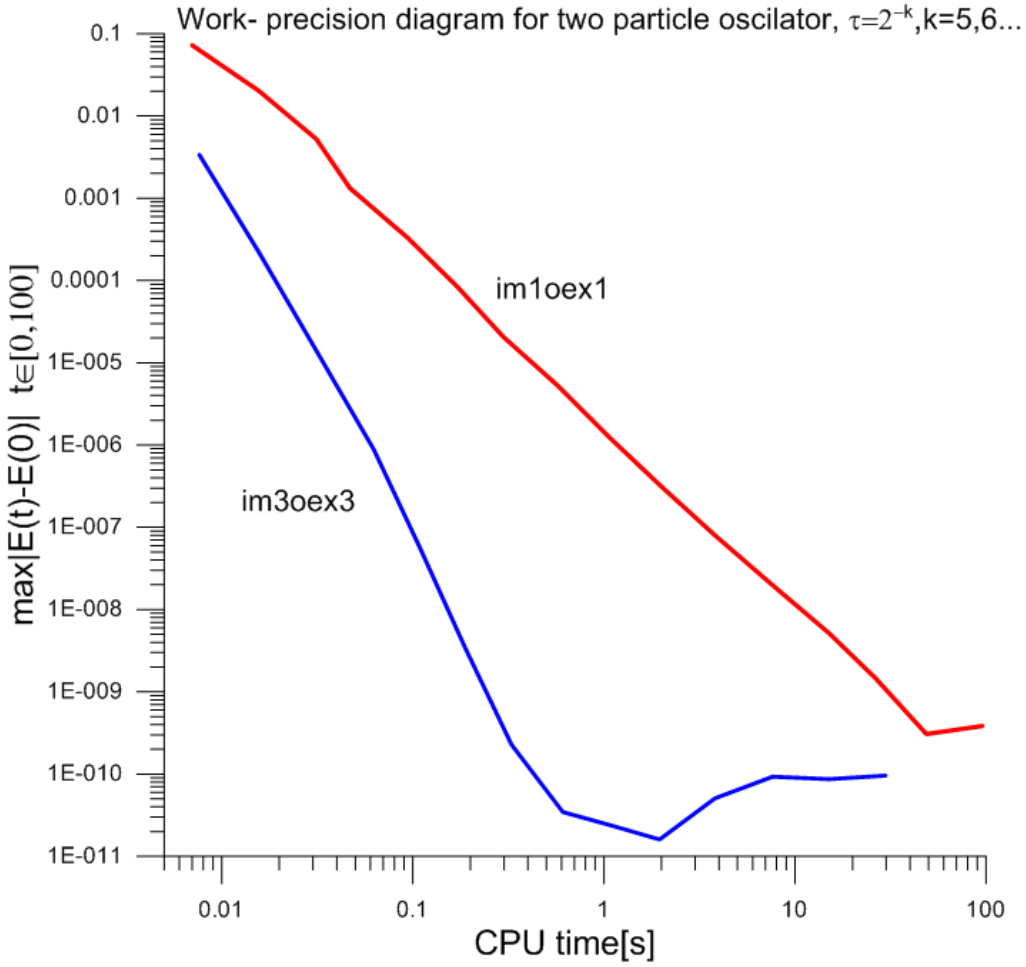
Long time integration for 12 particles in 8x8 box, $Im3 \circ Ex3$




Work- precision diagram for two particle oscilator, τ=2^-k,k=5,6...
max|E(t)-E(0)| t∈[0,100]
0.1
0.01
0.001
0.0001
1E-005
1E-006
1E-007
1E-008
1E-009
1E-010
1E-011
0.01
0.1
1
10
100
CPU time[s]
im1oex1
im3oex3