Step = 0

$\vec{r}_1^{\,0} = (0.75000000;\ 0.75000000;\ 0.50000000)$; $\vec{r}_2^{\,0} = (1.25000000;\ 0.75000000;\ 0.50000000)$;

$\vec{r}_{12}^{\,0} = (-0.50000000; 0.00000000; 0.00000000)$; $\vec{r}_{21}^{\,0} = (0.50000000; 0.00000000; 0.00000000)$;

$\left|\vec{r}_{12}^{\,0}\right| = 0.50000000$;

$U^0 = 111.54752063$;

$F_{12} = 10355.02043702$;

$\vec{F}_{12}{}^{0} = (\text{-}10355.02043702;\ 0.00000000;\ 0.00000000)$;
$\vec{F}_{21}{}^{0} = (10355.02043702;\ 0.00000000;\ 0.00000000)$;

$\vec{v}_1^{\,0} = (vx_1; vy_1; vz_1) = (1.00000000;\ 1.00000000;\ 0.00000000)$;

$\vec{v}_2^{\,0} = (vx_2; vy_2; vz_2) = (\text{-}1.00000000;\ 1.00000000;\ 0.00000000)$;

$E_{kin} = 398.01000000$

$E_{term} = 199.00500000$

$E_{pot} = \text{-}0.54622684$

$E_{int} = 198.45877316$

$E = 397.46377316$

$T = 48.04626134$

$P = 232.31334244$

Step = 1

$\vec{r}_1^{\,1} = (0.75189593;\ 0.75200000;\ 0.50000000)$; $\vec{r}_2^{\,1} = (1.24810407;\ 0.75200000;\ 0.50000000)$;

$\vec{r}_{12}^{\,1} = (-0.49620814;\ 0.00000000;\ 0.00000000)$; $\vec{r}_{21}^{\,1} = (0.49620814;\ 0.00000000;\ 0.00000000)$;

$\left|\vec{r}_{12}^{\,1}\right| = 0.49620814$;

$U^1 = 132.96912736$;

$F_{12} = 12487.60973912$;

$\vec{F}_{12}{}^{1} = (\text{-}12487.60973912;\ 0.00000000;\ 0.00000000)$;
$\vec{F}_{21}{}^{1} = (12487.60973912;\ 0.00000000;\ 0.00000000)$;

$\vec{v}_1^{\,1} = (vx_1; vy_1; vz_1) = (0.88521580;\ 1.00000000;\ 0.00000000)$;

$\vec{v}_2^{\,1} = (vx_2; vy_2; vz_2) = (\text{-}0.88521580;\ 1.00000000;\ 0.00000000)$;

$E_{kin} = 354.94671273$

$E_{term} = 155.94171273$

$E_{pot} = -0.56681568$

$E_{int} = 155.37489705$

$E = 354.37989705$

$T = 37.64938712$

$P = 271.18070732$

Step = 2

$\vec{r}_1^{\,3} = (0.75354086;\ 0.75400000;\ 0.50000000)$; $\vec{r}_2^{\,3} = (1.24645914;\ 0.75400000;\ 0.50000000)$;

$\vec{r}_{12}^{\,3} = (-0.49291827;\ 0.00000000;\ 0.00000000)$; $\vec{r}_{21}^{\,3} = (0.49291827;\ 0.00000000;\ 0.00000000)$;

$\left|\vec{r}_{12}^{\,3}\right| = 0.49291827$;

$U^3 = 154.79133278$;

$F_{12} = 14697.43005221$;

$\vec{F}_{12}{}^3 = (-14697.43005221;\ 0.00000000;\ 0.00000000)$;

$\vec{F}_{21}{}^3 = (14697.43005221;\ 0.00000000;\ 0.00000000)$;

$\vec{v}_1{}^3 = (vx_1; vy_1; vz_1) = (0.74861099;\ 1.00000000;\ 0.00000000)$;

$\vec{v}_2{}^3 = (vx_2; vy_2; vz_2) = (-0.74861099;\ 1.00000000;\ 0.00000000)$;

$E_{kin} = 310.53106650$

$E_{term} = 111.52606650$

$E_{pot} = -0.58527469$

$E_{int} = 110.94079181$

$E = 309.94579181$

$T = 26.92600959$

$P = 311.15349921$