







MD results:

flux1: flux through: -100000001.18000001

flux2: effective flux through: 1.1799999999999999

flux3: effective flux through: 1.1799999999999999

flux(ns)^1), error, relative error (%)

1	0.000000	0.000000	0.000000
2	0.000000	0.000000	0.000000
3	0.000000	0.000000	0.000000

MDcycles: 10000

NSA,NSB,NOSA,NSB 0 0 0 0

NCROSS 0 0 0

NEFFCROSS 0 0 0

NEFFCROSS/NCROSS NaN NaN

reactive flux correction: c1=NOSA/(MDcycles-NSB)

c1= 0.0000000000000000

flux1*c1,flux2*c1,flux3*c1:

0.000000 0.000000 0.000000

flux1: one effective crossing per Infinity timesteps

flux2: one effective crossing per Infinity timesteps

flux3: one effective crossing per Infinity timesteps

pMD1 0.0000000000000000 (1-p)/p Infinity

pMD2 0.0000000000000000 (1-p)/p Infinity

pMD3 0.0000000000000000 (1-p)/p Infinity

efficiency time 1 0.0000000000000000

efficiency time 2 0.0000000000000000

efficiency time 3 0.0000000000000000

correlation 1 0.0000000000000000

correlation 2 0.0000000000000000

correlation 3 0.0000000000000000

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transmission results: !! units might need a check!!!!!!!
trans_INTFL= -100000001.18000001
trans_INTFM=  1.1799999999999999
trans_INTFR=  1.1799999999999999
(unnormalized) kappa (A/ns), error, relative error (%)
      0.000000      0.000000      0.000000
(unnormalized) kappaTST (A/ns), error, relative error (%)
      0.000000      0.000000      0.000000
exact TST result  363.77042704416266
normalized kappa (k/kTST):  0.000000000000000000
num. integ. P_A(TS)=  0.000000000000000000      0.000000000000000000
reactive flux result rate
      0.000000000000000000      0.000000000000000000
two-point method:
      0.000000000000000000      0.000000000000000000

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TIS results

ensemble	1				
IL,IM,IR,Idetect	0.0000	0.0000	0.7000	0.0300	
pcross,err,rel. e(%)		0.272229	0.080463		29.556972
Lacc,Ltr, Ltr/Lacc		73.059601	38.032216		0.520564
TIScycles, Totsim	3104	118051.99999999999			
accRate, cor	0.70844072164948457		101.40097510664563		
teff	10313.194940617313				
ensemble	2				
IL,IM,IR,Idetect	0.0000	0.0300	0.7000	0.0700	
pcross,err,rel. e(%)		0.272229	0.089037		32.706721
Lacc,Ltr, Ltr/Lacc		200.729381	53.581186		0.266932
TIScycles, Totsim	3104	166316.00000000000			
accRate, cor	0.52673969072164950		124.16416120562262		
teff	17791.314497568852				
ensemble	3				
IL,IM,IR,Idetect	0.0000	0.0700	0.7000	0.1300	
pcross,err,rel. e(%)		0.116302	0.060501		52.020746
Lacc,Ltr, Ltr/Lacc		350.666881	81.937178		0.233661
TIScycles, Totsim	3104	254333.00000000000			
accRate, cor	0.44104381443298968		110.51375336468278		
teff	68826.529802570789				
ensemble	4				
IL,IM,IR,Idetect	0.0000	0.1300	0.7000	0.3100	
pcross,err,rel. e(%)		0.018686	0.009221		49.350316
Lacc,Ltr, Ltr/Lacc		527.573454	111.574420		0.211486
TIScycles, Totsim	3104	346327.00000000000			
accRate, cor	0.34826030927835050		14.389965492558082		
teff	84346.338260326389				
ensemble	5				
IL,IM,IR,Idetect	0.0000	0.3100	0.7000	0.3400	
pcross,err,rel. e(%)		0.048647	0.008708		17.899740
Lacc,Ltr, Ltr/Lacc		1649.226482	210.472938		0.127619
TIScycles, Totsim	3104	653308.00000000000			
accRate, cor	0.28060567010309279		5.0838029119104711		
teff	20932.032769020414				
ensemble	6				
IL,IM,IR,Idetect	0.0000	0.3400	0.7000	0.7000	
pcross,err,rel. e(%)		0.003222	0.000019		0.580467
Lacc,Ltr, Ltr/Lacc		2048.837629	305.448776		0.149084
TIScycles, Totsim	3104	948112.99999999988			
accRate, cor	0.52641752577319589		3.3792158294022959E-004		
teff	31.945858678719095				

additional PPS 000/001 results:

T0,err,rel.e(%)	4415.170829	673.916241	15.263650
T1,err,rel.e(%)	71.059601	7.240358	10.189134
LtrT0, Ltr/Lacc	2537.527806	0.574469	
LtrT1, Ltr/Lacc	38.032216	0.520564	
cyclesT0, Totsim	3003	7620196.0000000000	
cyclesT1, Totsim	3104	118051.9999999999	
accRateT0, cor	0.84082584082584078	11.718092692677027	
accRateT1, cor	0.70844072164948457	11.249513712169289	
teffT0	177534.58274593906		
teffT1	1225.5975917066194		

Combining all results:

flux= 218.95207974446259 +- 15.183272668301559 %
Pcross= 2.5240344903356297E-008 +- 86.056339557159546 %
rate= 5.5264260100574079E-006 +- 87.385498493154657 %

flux: sim.time, teff 7620196.0000000000 175669.72633970561
Pcross: sim.time, teff 2486449.0000000000 1841387.9391267688
Rate: sim.time, teff 10106645.0000000000 7717661.8721091188
Optimize Pcross teff: 879922.12138274824
Optimize rate teff: 1841914.1182033566
ratio of chosen NCYCLES
flux: 1.0000000000000000
TIS:

- 1 1.0336330336330337
- 2 1.0336330336330337
- 3 1.0336330336330337
- 4 1.0336330336330337
- 5 1.0336330336330337
- 6 1.0336330336330337

ratio of optimal NCYCLES
flux: 8.9262440856943979
TIS:

- 1 144.30324011935008
- 2 134.53113473008170
- 3 173.03264277466937
- 4 140.66938349109810
- 5 37.148436935446412
- 6 1.0000000000000000