```asm
.nb302_single_check:
        add dword ptr [rsp + nb302_innerk],  4
        jnz   .nb302_single_loop
        jmp   .nb302_updateouterdata
.nb302_single_loop:
        mov   rdx, [rsp + nb302_innerjjnr]        ;# pointer to jjnr[k]
        mov   eax, [rdx]
        add qword ptr [rsp + nb302_innerjjnr],  4

        mov rsi, [rbp + nb302_pos]
        lea   rax, [rax + rax*2]

        ;# fetch j coordinates
        xorps xmm0, xmm0
        xorps xmm1, xmm1
        xorps xmm2, xmm2

        movss xmm0, [rsi + rax*4]          ;# jxO  -  -  -
        movss xmm1, [rsi + rax*4 + 4]         ;# jyO  -  -  -
        movss xmm2, [rsi + rax*4 + 8]         ;# jzO  -  -  -

        movlps xmm6, [rsi + rax*4 + 12]        ;# xmm6 = jxH1 jyH1  -   -
        movss  xmm7, [rsi + rax*4 + 20]        ;# xmm7 = jzH1  -   -   -
        movhps xmm6, [rsi + rax*4 + 24]        ;# xmm6 = jxH1 jyH1 jxH2 jyH2
        movss  xmm5, [rsi + rax*4 + 32]        ;# xmm5 = jzH2  -   -   -

        ;# have all coords, time for some shuffling.

        shufps xmm6, xmm6, 216 ;# 11011000 ;# xmm6 = jxH1 jxH2 jyH1 jyH2
        unpcklps xmm7, xmm5                    ;# xmm7 = jzH1 jzH2  -   -

        movlhps xmm0, xmm6                     ;# xmm0 = jxO  0   jxH1 jxH2
        shufps  xmm1, xmm6, 228 ;# 11100100 ;# xmm1 = jyO  0   jyH1 jyH2
        shufps  xmm2, xmm7, 68  ;# 01000100 ;# xmm2 = jzO  0   jzH1 jzH2

        ;# store all j coordinates in jO
        movaps [rsp + nb302_jxO], xmm0
        movaps [rsp + nb302_jyO], xmm1
        movaps [rsp + nb302_jzO], xmm2
        subps  xmm0, [rsp + nb302_ixO]
        subps  xmm1, [rsp + nb302_iyO]
        subps  xmm2, [rsp + nb302_izO]
        movaps [rsp + nb302_dxOO], xmm0
        movaps [rsp + nb302_dyOO], xmm1
        movaps [rsp + nb302_dzOO], xmm2
        mulps xmm0, xmm0
        mulps xmm1, xmm1
        mulps xmm2, xmm2
```

```
        addps xmm0, xmm1
        addps xmm0, xmm2          ;# have rsq in xmm0

        ;# do invsqrt
        rsqrtps xmm1, xmm0
        movaps  xmm2, xmm1
        mulps   xmm1, xmm1
        movaps  xmm3, [rsp + nb302_three]
        mulps   xmm1, xmm0
        subps   xmm3, xmm1
        mulps   xmm3, xmm2
        mulps   xmm3, [rsp + nb302_half] ;# rinv iO - j water

        movaps  xmm1, xmm3
        mulps   xmm1, xmm0        ;# xmm1=r
        movaps  xmm0, xmm3        ;# xmm0=rinv
        mulps  xmm1, [rsp + nb302_tsc]

        movhlps xmm2, xmm1
        cvttps2pi mm6, xmm1
        cvttps2pi mm7, xmm2       ;# mm6/mm7 contain lu indices
        cvtpi2ps xmm3, mm6
        cvtpi2ps xmm2, mm7
        movlhps  xmm3, xmm2
        subps    xmm1, xmm3       ;# xmm1=eps
        movaps xmm2, xmm1
        mulps  xmm2, xmm2         ;# xmm2=eps2
        pslld   mm6, 2
        pslld   mm7, 2

        movd ebx, mm6
        movd ecx, mm7
        psrlq mm7, 32
        movd edx, mm7             ;# table indices in ebx,ecx,edx

        mov rsi, [rbp + nb302_VFtab]

        movlps xmm5, [rsi + rbx*4]
        movlps xmm7, [rsi + rcx*4]
        movhps xmm7, [rsi + rdx*4] ;# got half coulomb table
        movaps xmm4, xmm5
        shufps xmm4, xmm7, 136  ;# 10001000
        shufps xmm5, xmm7, 221  ;# 11011101

        movlps xmm7, [rsi + rbx*4 + 8]
        movlps xmm3, [rsi + rcx*4 + 8]
        movhps xmm3, [rsi + rdx*4 + 8] ;# other half of coulomb table
        movaps xmm6, xmm7
```

```
shufps xmm6, xmm3, 136  ;# 10001000
shufps xmm7, xmm3, 221  ;# 11011101
;# coulomb table ready, in xmm4-xmm7
mulps  xmm6, xmm1        ;# xmm6=Geps
mulps  xmm7, xmm2        ;# xmm7=Heps2
addps  xmm5, xmm6
addps  xmm5, xmm7        ;# xmm5=Fp
mulps  xmm7, [rsp + nb302_two]        ;# two*Heps2

xorps  xmm3, xmm3
;# fetch charges to xmm3 (temporary)
movss   xmm3, [rsp + nb302_qqOO]
movhps  xmm3, [rsp + nb302_qqOH]

addps  xmm7, xmm6
addps  xmm7, xmm5 ;# xmm7=FF
mulps  xmm5, xmm1 ;# xmm5=eps*Fp
addps  xmm5, xmm4 ;# xmm5=VV
mulps  xmm5, xmm3 ;# vcoul=qq*VV
mulps  xmm3, xmm7 ;# fijC=FF*qq
;# at this point xmm5 contains vcoul and xmm3 fijC

addps  xmm5, [rsp + nb302_vctot]
movaps [rsp + nb302_vctot], xmm5
xorps  xmm2, xmm2
mulps  xmm3, [rsp + nb302_tsc]

subps  xmm2, xmm3
mulps  xmm0, xmm2

movaps xmm1, xmm0
movaps xmm2, xmm0

mulps   xmm0, [rsp + nb302_dxOO]
mulps   xmm1, [rsp + nb302_dyOO]
mulps   xmm2, [rsp + nb302_dzOO]
;# initial update for j forces
xorps   xmm3, xmm3
xorps   xmm4, xmm4
xorps   xmm5, xmm5
addps   xmm3, xmm0
addps   xmm4, xmm1
addps   xmm5, xmm2
movaps  [rsp + nb302_fjxO], xmm3
movaps  [rsp + nb302_fjyO], xmm4
movaps  [rsp + nb302_fjzO], xmm5
addps   xmm0, [rsp + nb302_fixO]
addps   xmm1, [rsp + nb302_fiyO]
```

```asm
        addps   xmm2, [rsp + nb302_fizO]
        movaps  [rsp + nb302_fixO], xmm0
        movaps  [rsp + nb302_fiyO], xmm1
        movaps  [rsp + nb302_fizO], xmm2


        ;# done with i O Now do i H1 & H2 simultaneously first get i particle coords:
movaps  xmm0, [rsp + nb302_jxO]
movaps  xmm1, [rsp + nb302_jyO]
movaps  xmm2, [rsp + nb302_jzO]
movaps  xmm3, xmm0
movaps  xmm4, xmm1
movaps  xmm5, xmm2
        subps   xmm0, [rsp + nb302_ixH1]
        subps   xmm1, [rsp + nb302_iyH1]
        subps   xmm2, [rsp + nb302_izH1]
        subps   xmm3, [rsp + nb302_ixH2]
        subps   xmm4, [rsp + nb302_iyH2]
        subps   xmm5, [rsp + nb302_izH2]
        movaps [rsp + nb302_dxH1O], xmm0
        movaps [rsp + nb302_dyH1O], xmm1
        movaps [rsp + nb302_dzH1O], xmm2
        movaps [rsp + nb302_dxH2O], xmm3
        movaps [rsp + nb302_dyH2O], xmm4
        movaps [rsp + nb302_dzH2O], xmm5
        mulps xmm0, xmm0
        mulps xmm1, xmm1
        mulps xmm2, xmm2
        mulps xmm3, xmm3
        mulps xmm4, xmm4
        mulps xmm5, xmm5
        addps xmm0, xmm1
        addps xmm4, xmm3
        addps xmm0, xmm2         ;# have rsqH1 in xmm0
        addps xmm4, xmm5         ;# have rsqH2 in xmm4

        ;# start with H1, save H2 data
        movaps [rsp + nb302_rsqH2O], xmm4

        ;# do invsqrt
        rsqrtps xmm1, xmm0
        rsqrtps xmm5, xmm4
        movaps  xmm2, xmm1
        movaps  xmm6, xmm5
        mulps   xmm1, xmm1
        mulps   xmm5, xmm5
        movaps  xmm3, [rsp + nb302_three]
        movaps  xmm7, xmm3
```

```
        mulps   xmm1, xmm0
        mulps   xmm5, xmm4
        subps   xmm3, xmm1
        subps   xmm7, xmm5
        mulps   xmm3, xmm2
        mulps   xmm7, xmm6
        mulps   xmm3, [rsp + nb302_half] ;# rinv H1 - j water
        mulps   xmm7, [rsp + nb302_half] ;# rinv H2 - j water

        ;# start with H1, save H2 data
        movaps [rsp + nb302_rinvH2O], xmm7

        movaps xmm1, xmm3
        mulps  xmm1, xmm0          ;# xmm1=r
        movaps xmm0, xmm3          ;# xmm0=rinv
        mulps  xmm1, [rsp + nb302_tsc]

        movhlps xmm2, xmm1
        cvttps2pi mm6, xmm1
        cvttps2pi mm7, xmm2        ;# mm6/mm7 contain lu indices
        cvtpi2ps xmm3, mm6
        cvtpi2ps xmm2, mm7
        movlhps  xmm3, xmm2
        subps    xmm1, xmm3        ;# xmm1=eps
        movaps xmm2, xmm1
        mulps  xmm2, xmm2          ;# xmm2=eps2
        pslld   mm6, 2
        pslld   mm7, 2

        movd ebx, mm6
        movd ecx, mm7
        psrlq mm7, 32
        movd edx, mm7              ;# table indices in ebx,ecx,edx

        movlps xmm5, [rsi + rbx*4]
        movlps xmm7, [rsi + rcx*4]
        movhps xmm7, [rsi + rdx*4] ;# got half coulomb table
        movaps xmm4, xmm5
        shufps xmm4, xmm7, 136  ;# 10001000
        shufps xmm5, xmm7, 221  ;# 11011101

        movlps xmm7, [rsi + rbx*4 + 8]
        movlps xmm3, [rsi + rcx*4 + 8]
        movhps xmm3, [rsi + rdx*4 + 8] ;# other half of coulomb table
        movaps xmm6, xmm7
        shufps xmm6, xmm3, 136  ;# 10001000
        shufps xmm7, xmm3, 221  ;# 11011101
        ;# coulomb table ready, in xmm4-xmm7
```

```
    mulps  xmm6, xmm1          ;# xmm6=Geps
    mulps  xmm7, xmm2          ;# xmm7=Heps2
    addps  xmm5, xmm6
    addps  xmm5, xmm7          ;# xmm5=Fp
    mulps  xmm7, [rsp + nb302_two]          ;# two*Heps2

    xorps  xmm3, xmm3
    ;# fetch charges to xmm3 (temporary)
    movss   xmm3, [rsp + nb302_qqOH]
    movhps  xmm3, [rsp + nb302_qqHH]

    addps  xmm7, xmm6
    addps  xmm7, xmm5 ;# xmm7=FF
    mulps  xmm5, xmm1 ;# xmm5=eps*Fp
    addps  xmm5, xmm4 ;# xmm5=VV
    mulps  xmm5, xmm3 ;# vcoul=qq*VV
    mulps  xmm3, xmm7 ;# fijC=FF*qq
    ;# at this point xmm5 contains vcoul and xmm3 fijC
    addps  xmm5, [rsp + nb302_vctot]
    movaps [rsp + nb302_vctot], xmm5

xorps  xmm1, xmm1

    mulps xmm3, [rsp + nb302_tsc]
    mulps xmm3, xmm0
    subps  xmm1, xmm3

    movaps  xmm0, xmm1
    movaps  xmm2, xmm1
    mulps   xmm0, [rsp + nb302_dxH1O]
    mulps   xmm1, [rsp + nb302_dyH1O]
    mulps   xmm2, [rsp + nb302_dzH1O]
    ;# update forces H1 - j water
    movaps  xmm3, [rsp + nb302_fjxO]
    movaps  xmm4, [rsp + nb302_fjyO]
    movaps  xmm5, [rsp + nb302_fjzO]
    addps   xmm3, xmm0
    addps   xmm4, xmm1
    addps   xmm5, xmm2
    movaps  [rsp + nb302_fjxO], xmm3
    movaps  [rsp + nb302_fjyO], xmm4
    movaps  [rsp + nb302_fjzO], xmm5
    addps   xmm0, [rsp + nb302_fixH1]
    addps   xmm1, [rsp + nb302_fiyH1]
    addps   xmm2, [rsp + nb302_fizH1]
    movaps  [rsp + nb302_fixH1], xmm0
    movaps  [rsp + nb302_fiyH1], xmm1
    movaps  [rsp + nb302_fizH1], xmm2
```

```
;# do table for H2 - j water interaction
movaps xmm0, [rsp + nb302_rinvH2O]
movaps xmm1, [rsp + nb302_rsqH2O]
mulps  xmm1, xmm0         ;# xmm0=rinv, xmm1=r
mulps  xmm1, [rsp + nb302_tsc]

movhlps xmm2, xmm1
cvttps2pi mm6, xmm1
cvttps2pi mm7, xmm2       ;# mm6/mm7 contain lu indices
cvtpi2ps xmm3, mm6
cvtpi2ps xmm2, mm7
movlhps  xmm3, xmm2
subps    xmm1, xmm3       ;# xmm1=eps
movaps xmm2, xmm1
mulps  xmm2, xmm2         ;# xmm2=eps2
pslld   mm6, 2
pslld   mm7, 2

movd ebx, mm6
movd ecx, mm7
psrlq mm7, 32
movd edx, mm7             ;# table indices in ebx,ecx,edx

movlps xmm5, [rsi + rbx*4]
movlps xmm7, [rsi + rcx*4]
movhps xmm7, [rsi + rdx*4] ;# got half coulomb table
movaps xmm4, xmm5
shufps xmm4, xmm7, 136  ;# 10001000
shufps xmm5, xmm7, 221  ;# 11011101

movlps xmm7, [rsi + rbx*4 + 8]
movlps xmm3, [rsi + rcx*4 + 8]
movhps xmm3, [rsi + rdx*4 + 8] ;# other half of coulomb table
movaps xmm6, xmm7
shufps xmm6, xmm3, 136  ;# 10001000
shufps xmm7, xmm3, 221  ;# 11011101
;# coulomb table ready, in xmm4-xmm7
mulps  xmm6, xmm1         ;# xmm6=Geps
mulps  xmm7, xmm2         ;# xmm7=Heps2
addps  xmm5, xmm6
addps  xmm5, xmm7         ;# xmm5=Fp
mulps  xmm7, [rsp + nb302_two]         ;# two*Heps2

xorps  xmm3, xmm3
;# fetch charges to xmm3 (temporary)
movss   xmm3, [rsp + nb302_qqOH]
movhps  xmm3, [rsp + nb302_qqHH]
```

```asm
        addps  xmm7, xmm6
        addps  xmm7, xmm5 ;# xmm7=FF
        mulps  xmm5, xmm1 ;# xmm5=eps*Fp
        addps  xmm5, xmm4 ;# xmm5=VV
        mulps  xmm5, xmm3 ;# vcoul=qq*VV
        mulps  xmm3, xmm7 ;# fijC=FF*qq
        ;# at this point xmm5 contains vcoul and xmm3 fijC
        addps  xmm5, [rsp + nb302_vctot]
        movaps [rsp + nb302_vctot], xmm5

xorps  xmm1, xmm1

        mulps xmm3, [rsp + nb302_tsc]
        mulps xmm3, xmm0
        subps  xmm1, xmm3

        movaps  xmm0, xmm1
        movaps  xmm2, xmm1

        mulps   xmm0, [rsp + nb302_dxH2O]
        mulps   xmm1, [rsp + nb302_dyH2O]
        mulps   xmm2, [rsp + nb302_dzH2O]
        movaps  xmm3, [rsp + nb302_fjxO]
        movaps  xmm4, [rsp + nb302_fjyO]
        movaps  xmm5, [rsp + nb302_fjzO]
        addps   xmm3, xmm0
        addps   xmm4, xmm1
        addps   xmm5, xmm2
        mov     rsi, [rbp + nb302_faction]
        movaps [rsp + nb302_fjxO], xmm3
        movaps [rsp + nb302_fjyO], xmm4
        movaps [rsp + nb302_fjzO], xmm5
        addps   xmm0, [rsp + nb302_fixH2]
        addps   xmm1, [rsp + nb302_fiyH2]
        addps   xmm2, [rsp + nb302_fizH2]
        movaps [rsp + nb302_fixH2], xmm0
        movaps [rsp + nb302_fiyH2], xmm1
        movaps [rsp + nb302_fizH2], xmm2

        ;# update j water forces from local variables
        movlps  xmm0, [rsi + rax*4]
        movlps  xmm1, [rsi + rax*4 + 12]
        movhps  xmm1, [rsi + rax*4 + 24]
        movaps  xmm3, [rsp + nb302_fjxO]
        movaps  xmm4, [rsp + nb302_fjyO]
        movaps  xmm5, [rsp + nb302_fjzO]
        movaps  xmm6, xmm5
        movaps  xmm7, xmm5
```

```asm
        shufps  xmm6, xmm6, 2 ;# 00000010
        shufps  xmm7, xmm7, 3 ;# 00000011
        addss   xmm5, [rsi + rax*4 + 8]
        addss   xmm6, [rsi + rax*4 + 20]
        addss   xmm7, [rsi + rax*4 + 32]
        movss   [rsi + rax*4 + 8], xmm5
        movss   [rsi + rax*4 + 20], xmm6
        movss   [rsi + rax*4 + 32], xmm7
        movaps   xmm5, xmm3
        unpcklps xmm3, xmm4
        unpckhps xmm5, xmm4
        addps    xmm0, xmm3
        addps    xmm1, xmm5
        movlps  [rsi + rax*4], xmm0
        movlps  [rsi + rax*4 + 12], xmm1
        movhps  [rsi + rax*4 + 24], xmm1

        dec dword ptr [rsp + nb302_innerk]
        jz    .nb302_updateouterdata
        jmp   .nb302_single_loop
```