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Summary of Multipole Component Variables & Expressions in Tinker

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Math Operations and Symbolic Notation

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dot vector dot/inner product (scalar, sum of 3 pair products)

crx vector cross/outer product (vector)

ddot "tensor double dot product" (scalar, sum of 9 pair products)

[] significance of variable

{} variable name of older versions of Tinker

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Sites Equivalence in Code

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ii first multipole [site number]

i ipole(i) [atom number]

xi x(i) [x-coordinate]

yi y(i) [y-coordinate]

zi z(i) [z-coordinate]

kk second multipole [site number]

k ipole(k) [atom number]

xk x(k) [x-coordinate]

yk y(k) [y-coordinate]

zk z(k) [z-coordinate]

xr xk - xi [x-distance]

yr yk - yi [y-distance]

zr zk - zi [z-distance]

###### ###################

Mpoles Equivalence in Code

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ci rpole(1,ii) [monopole]

dix rpole(2,ii) [x-dipole]

diy rpole(3,ii) [y-dipole]

diz rpole(4,ii) [z-dipole]

qixx rpole(5,ii) [xx-quadrupole]

qixy rpole(6,ii) [xy-quadrupole]

qixz rpole(7,ii) [xz-quadrupole]

qiyy rpole(8,ii) [yy-quadrupole]

qiyz rpole(9,ii) [yz-quadrupole]

qizz rpole(10,ii) [zz-quadrupole]

uix uind(1,ii) [x-induced]

uiy uind(2,ii) [y-induced]

uiz uind(3,ii) [z-induced]

ck rpole(1,kk) [monopole]

dkx rpole(2,kk) [x-dipole]

dky rpole(3,kk) [y-dipole]

dkz rpole(4,kk) [z-dipole]

qkxx rpole(5,kk) [xx-quadrupole]

qkxy rpole(6,kk) [xy-quadrupole]

qkxz rpole(7,kk) [xz-quadrupole]

qkyy rpole(8,kk) [yy-quadrupole]

qkyz rpole(9,kk) [yz-quadrupole]

qkzz rpole(10,kk) [zz-quadrupole]

ukx uind(1,kk) [x-induced]

uky uind(2,kk) [y-induced]

ukz uind(3,kk) [z-induced]

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Energy Equivalence in Code

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dir dix\*xr + diy\*yr + diz\*zr [di-dot-r] {dri}

qix qixx\*xr + qixy\*yr + qixz\*zr [qix-dot-r] {qrix}

qiy qixy\*xr + qiyy\*yr + qiyz\*zr [qiy-dot-r] {qriy}

qiz qixz\*xr + qiyz\*yr + qizz\*zr [qiz-dot-r] {qriz}

qir qix\*xr + qiy\*yr + qiz\*zr [qi-dot-r] {qrri}

dkr dkx\*xr + dky\*yr + dkz\*zr [dk-dot-r] {drk}

qkx qkxx\*xr + qkxy\*yr + qkxz\*zr [qkx-dot-r] {qrkx}

qky qkxy\*xr + qkyy\*yr + qkyz\*zr [qky-dot-r] {qrky}

qkz qkxz\*xr + qkyz\*yr + qkzz\*zr [qkz-dot-r] {qrkz}

qkr qkx\*xr + qky\*yr + qkz\*zr [qk-dot-r] {qrrk}

dik dix\*dkx + diy\*dky + diz\*dkz [di-dot-dk] {dik}

qik qix\*qkx + qiy\*qky + qiz\*qkz [qi-dot-qk] {qrrik}

diqk dix\*qkx + diy\*qky + diz\*qkz [di-dot-qk] {diqrk}

dkqi dkx\*qix + dky\*qiy + dkz\*qiz [dk-dot-qi] {dkqri}

qiqk 2.0d0\*(qixy\*qkxy+qixz\*qkxz+qiyz\*qkyz) [qi-ddot-qk] {qik}

+ qixx\*qkxx + qiyy\*qkyy + qizz\*qkzz

diu dix\*ukx + diy\*uky + diz\*ukz [di-dot-uk] {duik}\*

qiu qix\*ukx + qiy\*uky + qiz\*ukz [qi-dot-uk] {quik)\*

uir uix\*xr + uiy\*yr + uiz\*zr [ui-dot-r] {uri}

dku dkx\*uix + dky\*uiy + dkz\*uiz [dk-dot-ui] {duik}\*

qku qkx\*uix + qky\*uiy + qkz\*uiz [qk-dot-ui] {quik)\*

ukr ukx\*xr + uky\*yr + ukz\*zr [uk-dot-r] {urk}

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Gradient Equivalence in Code

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dirx diy\*zr - diz\*yr [x of di-crs-r] {dirx}

diry diz\*xr - dix\*zr [y of di-crs-r] {diry}

dirz dix\*yr - diy\*xr [z of di-crs-r] {dirz}

dkrx dky\*zr - dkz\*yr [x of dk-crs-r] {dkrx}

dkry dkz\*xr - dkx\*zr [y of dk-crs-r] {dkry}

dkrz dkx\*yr - dky\*xr [z of dk-crs-r] {dkrz}

dikx diy\*dkz - diz\*dky [x of di-crs-dk] {dikx}

diky diz\*dkx - dix\*dkz [y of di-crs-dk] {diky}

dikz dix\*dky - diy\*dkx [z of di-crs-dk] {dikz}

qirx qiz\*yr - qiy\*zr [x of qi-crs-r] {qrixr}

qiry qix\*zr - qiz\*xr [y of qi-crs-r] {qriyr}

qirz qiy\*xr - qix\*yr [z of qi-crs-r] {qrizr}

qkrx qkz\*yr - qky\*zr [x of qk-crs-r] {qrkxr}

qkry qkx\*zr - qkz\*xr [y of qk-crs-r] {qrkyr}

qkrz qky\*xr - qkx\*yr [z of qk-crs-r] {qrkzr}

qikx qky\*qiz - qkz\*qiy [x of qi-crs-qk] {qrrx}

qiky qkz\*qix - qkx\*qiz [y of qi-crs-qk] {qrry}

qikz qkx\*qiy - qky\*qix [z of qi-crs-qk] {qrrz}

qixk qixx\*qkx + qixy\*qky + qixz\*qkz [qix's-dot-qk] {qikrx}

qiyk qixy\*qkx + qiyy\*qky + qiyz\*qkz [qiy's-dot-qk] {qikry}

qizk qixz\*qkx + qiyz\*qky + qizz\*qkz [qiz's-dot-qk] {qikrz}

qkxi qkxx\*qix + qkxy\*qiy + qkxz\*qiz [qkx's-dot-qi] {qkirx}

qkyi qkxy\*qix + qkyy\*qiy + qkyz\*qiz [qiy's-dot-qk] {qikry}

qkzi qkxz\*qix + qkyz\*qiy + qkzz\*qiz [qiz's-dot-qk] {qikrz}

qikrx qizk\*yr - qiyk\*zr [x of qik-crs-r] {qikrxr}

qikry qixk\*zr - qizk\*xr [y of qik-crs-r] {qikryr}

qikrz qiyk\*xr - qixk\*yr [z of qik-crs-r] {qikrzr}

qkirx qkzi\*yr - qkyi\*zr [x of qki-crs-r] {qkirxr}

qkiry qkxi\*zr - qkzi\*xr [y of qki-crs-r] {qkiryr}

qkirz qkyi\*xr - qkxi\*yr [z of qki-crs-r] {qkirzr}

diqkx dix\*qkxx + diy\*qkxy + diz\*qkxz [di-dot-qkx's] {diqkx}

diqky dix\*qkxy + diy\*qkyy + diz\*qkyz [di-dot-qky's] {diqky}

diqkz dix\*qkxz + diy\*qkyz + diz\*qkzz [di-dot-qkz's] {diqkz}

dkqix dkx\*qixx + dky\*qixy + dkz\*qixz [dk-dot-qix's] {dkqix}

dkqiy dkx\*qixy + dky\*qiyy + dkz\*qiyz [dk-dot-qiy's] {dkqiy}

dkqiz dkx\*qixz + dky\*qiyz + dkz\*qizz [dk-dot-qiz's] {dkqiz}

diqkrx diqkz\*yr - diqky\*zr [x of diqk-crs-r] {diqkxr}

diqkry diqkx\*zr - diqkz\*xr [x of diqk-crs-r] {diqkyr}

diqkrz diqky\*xr - diqkx\*yr [x of diqk-crs-r] {diqkzr}

dkqirx dkqiz\*yr - dkqiy\*zr [x of dkqi-crs-r] {dkqixr}

dkqiry dkqix\*zr - dkqiz\*xr [y of dkqi-crs-r] {dkqiyr}

dkqirz dkqiy\*xr - dkqix\*yr [z of dkqi-crs-r] {dkqizr}

dqikx diy\*qkz - diz\*qky + dky\*qiz - dkz\*qiy [complex] {dqiqkx}

- 2.0d0\*(qixy\*qkxz+qiyy\*qkyz+qiyz\*qkzz

-qixz\*qkxy-qiyz\*qkyy-qizz\*qkyz)

dqiky diz\*qkx - dix\*qkz + dkz\*qix - dkx\*qiz [complex] {dqiqky}

- 2.0d0\*(qixz\*qkxx+qiyz\*qkxy+qizz\*qkxz

-qixx\*qkxz-qixy\*qkyz-qixz\*qkzz)

dqikz dix\*qky - diy\*qkx + dkx\*qiy - dky\*qix [complex] {dqiqkz}

- 2.0d0\*(qixx\*qkxy+qixy\*qkyy+qixz\*qkyz

-qixy\*qkxx-qiyy\*qkxy-qiyz\*qkxz)