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<pre>%Buneman, O., TRISTAN: The 3-D E-M Particle Code, in {\it Computer Space Plasma % Physics: Simulation Techniques and Software}, ed. H. Matsumoto and Y. % Omura, P.67, 1993. common /partls/ x(8192),y(8192),z(8192),u(8192),v(8192),w(8192) common /fields/ exl(8192),eyl(8192),ezl(8192), &bxl(8192),byl(8192),bzl(8192) dimension smooth(30),mooths(30) equivalence (smooth(28),rs),(smooth(29),ps),(smooth(30),qs), &(mooths(28),ix),(mooths(29),iy),(mooths(30),iz) real me,mi C Fields can be treated as single-indexed or triple-indexed: dimension ex(21,19,20),ey(21,19,20),ez(21,19,20), &bx(21,19,20),by(21,19,20),bz(21,19,20) equivalence (exl(1),ex(1,1,1)), (eyl(1),ey(1,1,1)), (ezl(1),ez(1, &l,1)), (bxl(1),bx(1,1,1)), (byl(1),by(1,1,1)), (bzl(1),bz(1,1,1)), &(ezl(8001),c),(ezl(8002),q),(ezl(8003),smooth(1)), &(ezl(8033),mooths(1)) dimension rho(21,19,20) equivalence (x(97),rho(1,1,1)) C For CRAY-s, the first two field dimensions should be ODD, as here: mx=21 my=19 mz=20 C Strides for single-indexed field arrays: ix=1 iy=mx iz=iy*my lot=iz*mz C Miscellaneous constants: qe=-1. qi=1. me=1. mi=32. qme=qe/me qmi=qi/mi c=.5 C Our finite difference equations imply delta_t = delta_x = C delta_y = delta_z = 1. So c must satisfy the Courant condition. C The bx,by and bz arrays are really records of c*Bx, c*By, C c*Bz: this makes for e <-----> b symmetry in Maxwell's equations. C In the particle arrays the ions are at the bottom, the electrons C are stacked against the top, the total number not exceeding maxptl: maxptl=8192 C ions=3700 C lecs=4300 C These are sample values for the number of ions, "ions", and the number C of electrons, "lecs". The initialiser (see below) may change them. C The code treats unpaired electrons as having been initially C dissociated from infinitely heavy ions which remain in situ. C In general the total information for particles will be somewhat C larger than that for fields. The limit "8192" per component is C used here for convenience of fitting the data into a segmented C PC memory. C For use in the boundary field calculation: rs=(1.-c)/(1.+c) tsq=.1666667 ps=r*(1.-tsq) qs=.5*r*(1.+tsq) C Data for smoothing: the currents fed into Maxwell's equations C are smoothed by convolving with the sequence .25, .5, .25 in C each dimension. Generate the 27 weights ("smooth") and index C displacements ("mooths"): n=1 do 1 nz=-1,1 do 1 ny=-1,1 do 1 nx=-1,1 smooth(n)=.015625*(2-nx*nx)*(2-ny*ny)*(2-nz*nz) mooths(n)=ix*nx+iy*ny+iz*nz</pre>		
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<pre>1 n=n+1 C Initialise the particles: Place electrons in same locations as ions C for zero initial net charge density. Keep particles 2 units away from C the boundaries of the field domain. Here we populate the interior of C a sphere (radius 7.75 and centered in the field domain) uniformly C with ion-electron pairs: rsq=60. C Place ions within sphere on cubic grid: CC ions=0 CC nzmax=sqrt(rsq) CC do 2 nz=-nzmax,nzmax CC nymax=sqrt(rsq-nz*nz) CC do 2 ny=-nymax,nymax CC nxmax=sqrt(rsq-nz*nz-ny*ny) CC do 2 nx=-nxmax,nxmax CC ions=ions+1 CC x(ions)=11.+nx CC y(ions)=10.+ny CC2 z(ions)=10.5+nz C Place ions within sphere on interstitial grid (cube centers): CC nzmax=-1+2*ifix(.5+sqrt(rsq)) CC do 3 nz=-nzmax,nzmax,2 CC nymax=-1+2*ifix(.5+sqrt(rsq-.25*nz*nz)) CC do 3 ny=-nymax,nymax,2 CC nxmax=-1+2*ifix(.5+sqrt(rsq-.25*nz*nz-.25*ny*ny)) CC do 3 nx=-nxmax,nxmax,2 CC ions=ions+1 CC x(ions)=11.+5*nx CC y(ions)=10.+5*ny CC3 z(ions)=10.5+5*nz CC open(6,file='con') CC write(6,97)ions CC97 format(i6) C As another example, fill one cell uniformly with 64 pairs: ions=0 do 80 k=1,4 do 80 j=1,4 do 80 i=1,4 ions=ions+1 x(ions)=11.375+.25*i y(ions)=10.375+.25*j 80 z(ions)=11.375+.25*k C Put electrons in the same places: lecs=ions do 4 n=1,lecs x(n+maxptl-lecs)=x(n) y(n+maxptl-lecs)=y(n) 4 z(n+maxptl-lecs)=z(n) C Since "ions" is less than 4096 in these cases, there would be room C for more particles. For instance, several hundred unpaired electrons C could be added at the bottom of the electron array. C Initialise velocities: these should not exceed c in magnitude! C For thermal distributions, add four random numbers for each C component and scale. In this test we use c for each component (too much!): do 85 n=1,ions u(n)=-0.5 v(n)=-0.5 w(n)=-0.5 u(maxptl-lecs+n)=0.5 v(maxptl-lecs+n)=0.5 85 w(maxptl-lecs+n)=0.5 C Initialise the fields, typically to uniform components, such as C just a uniform magnetic field parallel to the z-axis. Here we create C linearly varying fields, the E-field curl-free as if static and both C E and B divergence-free: do 5 k=1,mz do 5 j=1,my do 5 i=1,mx ex(i,j,k)=.001*(i-10.5)-.005*(j-10.0)-.004*(k-10.5)</pre>		

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	<pre> & (by(i,j,k-1)-by(i,j,k)-bz(i,j-1,k)+bz(i,j,k)) ey(i,j,k)=ey(i,j,k) + c * & (bz(i-1,j,k)-bz(i,j,k)-bx(i,j,k-1)+bx(i,j,k)) 9 ez(i,j,k)=ez(i,j,k) + c * & (bx(i,j-1,k)-bx(i,j,k)-by(i-1,j,k)+by(i,j,k)) C Boundary values of the E - field must be provided at rear, left C and bottom faces of the field domain: call surface(ex,ey,ez,bx,by,bz,-ix,-iy,-iz,mx,my,mz,lot) call surface(ey,ez,ex,by,bz,bx,-iy,-iz,-ix,my,mz,mx,lot) call surface(ez,ex,ey,bz,bx,by,-iz,-ix,-iy,mz,mx,my,lot) call edge(ex,-ix,-iy,-iz,mx,my,mz,lot) call edge(ey,-iy,-iz,-ix,my,mz,mx,lot) call edge(ez,-iz,-ix,-iy,mz,mx,my,lot) C The currents due to the movement of each charge q are applied to the C E-M fields as decrements of E-flux through cell faces. The movement C of particles which themselves cross cell boundaries has to be split C into several separate moves, each only within one cell. Each of C these moves contributes to flux across twelve faces. C Ions and electrons are processed in two loops, changing the sign C of the charge in-between. These loops cannot be vectorised: C particles get processed on by one. Here is a good place to C insert the "if" clauses for applying boundary conditions to C the particles, such as reflection, periodicity, replacement C by inward moving thermal or streaming particles, etc. q=qi do 10 n=1,ions 10 call usplit(x(n),y(n),z(n),u(n),v(n),w(n)) q=qe do 11 n=maxptl-lecs+1,maxptl 11 call usplit(x(n),y(n),z(n),u(n),v(n),w(n)) C These "split" routines call the deposit routine. C Countdown: nstep=nstep+1 if (nstep.le.last) go to 6 CC divergence check: do 75 k=2,mz do 75 j=2,my do 75 i=2,mx 75 rho(i,j,k)=ex(i,j,k)-ex(i-1,j,k)+ey(i,j,k)-ey(i,j-1,k) & +ez(i,j,k)-ez(i,j,k-1) write(*,'(16f5.1)')((rho(i,j,k),i=8,15),j=7,14),k=8,15) CC end of divergence check CC write(*,'(6h ions:)'') CC write(*,'(16f5.2)')(x(n),n=1,ions),(y(n),n=1,ions),(z(n),n=1,ions) CC write(*,'(6h lecs:)'') CC write(*,'(16f5.2)')(x(n),n=maxptl-lecs+1,maxptl), CC & (y(n),n=maxptl-lecs+1,maxptl), CC & (z(n),n=maxptl-lecs+1,maxptl) stop end C ----- subroutine surface(bx,by,bz,ex,ey,ez,ix,iy,iz,mx,my,mz,m00) dimension bx(1),by(1),bz(1),ex(1),ey(1),ez(1) common /fields/ ex0(8192),ey0(8192),ez0(8000),c,q0,smooth(27), &r,p,q,dummy(160),bx0(8192),by0(8192),bz0(8192) m0=m00+iz*(mz-1) assign 5 to next 6 m=m0 do 2 j=1,my-1 n=m do 1 i=1,mx-1 bz(n)=bz(n)+.5*c*(ex(n+iy)-ex(n)-ey(n+ix)+ey(n)) 1 n=n+ix 2 m=m+iy go to next (5,7) 7 return 5 m=m0+ix+iy do 4 j=2,my-1 n=m </pre>	

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	<pre> C Directive specifically for the CRAY cft77 compiler: cdirc\$ ivdep do 3 i=2,mx-1 bx(n)=bx(n-iz)+r*(bx(n)-bx(n-iz))+p*(bz(n)-bz(n-ix))-q*(ez(n+iy)- &ez(n))-(q-c)*(ez(n+iy-iz)-ez(n-iz))-c*(ey(n)-ey(n-iz)) by(n)=by(n-iz)+r*(by(n)-by(n-iz))+p*(bz(n)-bz(n-iy))+q*(ez(n+ix)- &ez(n))+(q-c)*(ez(n+ix-iz)-ez(n-iz))+c*(ex(n)-ex(n-iz)) 3 n=n+ix 4 m=m+iy assign 7 to next go to 6 end C ----- subroutine edge(bx,ix,iy,iz,mx,my,mz,m00) dimension bx(1) lx=ix*(mx-1) ly=iy*(my-1) lz=iz*(mz-1) n=m00+iy+lz cdirc\$ ivdep do 1 j=2,my-1 bx(n)=bx(n+ix)+bx(n-iz)-bx(n+ix-iz) bx(n+lx)=bx(n+lx-ix)+bx(n+lx-iz)-bx(n+lx-ix-iz) 1 n=n+iy n=m00+ly+iz cdirc\$ ivdep do 2 k=2,mz-1 bx(n)=bx(n+ix)+bx(n-iy)-bx(n+ix-iy) bx(n+lx)=bx(n+lx-ix)+bx(n+lx-iy)-bx(n+lx-ix-iy) 2 n=n+iz n=m00+ly+lz cdirc\$ ivdep do 3 i=1,mx bx(n)=bx(n-iy)+bx(n-iz)-bx(n-iy-iz) bx(n-ly)=bx(n-ly+iy)+bx(n-ly-iz)-bx(n-ly+iy-iz) bx(n-lz)=bx(n-lz-iy)+bx(n-lz+iz)-bx(n-lz-iy+iz) 3 n=n+ix return end C----- subroutine mover(n1,n2,qm) common /partls/ x(8192),y(8192),z(8192),u(8192),v(8192),w(8192) common /fields/ ex(8192),ey(8192),ez(8192), &bx(8192),by(8192),bz(8192) dimension mooths(30) equivalence (ez(8001),c),(ez(8033),mooths(1)),(mooths(28),ix), &(mooths(29),iy),(mooths(30),iz) do 1 n=n1,n2 C Cell index & displacement in cell: i=x(n) dx=x(n)-i j=y(n) dy=y(n)-j k=z(n) dz=z(n)-k li=iy*(j-1)+iz*(k-1) C (Field components are treated as single-indexed in this subroutine) C Field interpolations are tri-linear (linear in x times linear in y C times linear in z). This amounts to the 3-D generalisation of "area C weighting". A modification of the simple linear interpolation formula C f(i+dx) = f(i) + dx * (f(i+1)-f(i)) C is needed since fields are recorded at half-integer locations in certain C dimensions: see comments and illustration with the Maxwell part of this C code. One then has first to interpolate from "midpoints" to "gridpoints" C by averaging neighbors. Then one proceeds with normal interpolation. C Combining these two steps leads to: C f at location i+dx = half of f(i)+f(i-1) + dx*(f(i+1)-f(i-1)) C where now f(i) means f at location i+1/2. The halving is absorbed C in the final scaling. </pre>	

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C	<i>E-component interpolations:</i> f=ex(l)+ex(l-ix)+dx*(ex(l+ix)-ex(l-ix)) f=f+dy*(ex(l+iy)+ex(l-ix+iy)+dx*(ex(l+ix+iy)-ex(l-ix+iy))-f) g=ex(l+iz)+ex(l-ix+iz)+dx*(ex(l+ix+iz)-ex(l-ix+iz)) g=g+dy* & (ex(l+iy+iz)+ex(l-ix+iy+iz)+dx*(ex(l+ix+iy+iz)-ex(l-ix+iy+iz))-g) ex0=(f+dz*(g-f))*(.25*qm)	
C	----- f=ey(l)+ey(l-iy)+dy*(ey(l+iy)-ey(l-iy)) f=f+dz*(ey(l+iz)+ey(l-iy+iz)+dy*(ey(l+iy+iz)-ey(l-iy+iz))-f) g=ey(l+ix)+ey(l-iy+ix)+dy*(ey(l+iy+ix)-ey(l-iy+ix)) g=g+dz* & (ey(l+iz+ix)+ey(l-iy+iz+ix)+dy*(ey(l+iy+iz+ix)-ey(l-iy+iz+ix))-g) ey0=(f+dx*(g-f))*(.25*qm)	
C	----- f=ez(l)+ez(l-iz)+dz*(ez(l+iz)-ez(l-iz)) f=f+dx*(ez(l+ix)+ez(l-iz+ix)+dz*(ez(l+iz+ix)-ez(l-iz+ix))-f) g=ez(l+iy)+ez(l-iz+iy)+dz*(ez(l+iz+iy)-ez(l-iz+iy)) g=g+dx* & (ez(l+ix+iy)+ez(l-iz+ix+iy)+dz*(ez(l+iz+ix+iy)-ez(l-iz+ix+iy))-g) ez0=(f+dy*(g-f))*(.25*qm)	
C	-----	
C	<i>B-component interpolations:</i> f=bx(l-iy)+bx(l-iy-iz)+dz*(bx(l-iy+iz)-bx(l-iy-iz)) f=bx(l)+bx(l-iz)+dz*(bx(l+iz)-bx(l-iz))+f+dy* & (bx(l+iy)+bx(l+iy-iz)+dz*(bx(l+iy+iz)-bx(l+iy-iz))-f) g=bx(l+ix-iy)+bx(l+ix-iy-iz)+dz*(bx(l+ix-iy+iz)-bx(l+ix-iy-iz)) g=bx(l+ix)+bx(l+ix-iz)+dz*(bx(l+ix+iz)-bx(l+ix-iz))+g+dy* & (bx(l+ix+iy)+bx(l+ix+iy-iz)+dz*(bx(l+ix+iy+iz)-bx(l+ix+iy-iz))-g) bx0=(f+dx*(g-f))*(.125*qm/c)	
C	----- f=by(l-iz)+by(l-iz-ix)+dx*(by(l-iz+ix)-by(l-iz-ix)) f=by(l)+by(l-ix)+dx*(by(l+ix)-by(l-ix))+f+dz* & (by(l+iz)+by(l+iz-ix)+dx*(by(l+iz+ix)-by(l+iz-ix))-f) g=by(l+iy-iz)+by(l+iy-iz-ix)+dx*(by(l+iy-iz+ix)-by(l+iy-iz-ix)) g=by(l+iy)+by(l+iy-ix)+dx*(by(l+iy+ix)-by(l+iy-ix))+g+dz* & (by(l+iy+iz)+by(l+iy+iz-ix)+dx*(by(l+iy+iz+ix)-by(l+iy+iz-ix))-g) by0=(f+dy*(g-f))*(.125*qm/c)	
C	----- f=bz(l-ix)+bz(l-ix-iy)+dy*(bz(l-ix+iy)-bz(l-ix-iy)) f=bz(l)+bz(l-iy)+dy*(bz(l+iy)-bz(l-iy))+f+dx* & (bz(l+ix)+bz(l+ix-iy)+dy*(bz(l+ix+iy)-bz(l+ix-iy))-f) g=bz(l+iz-ix)+bz(l+iz-ix-iy)+dy*(bz(l+iz-ix+iy)-bz(l+iz-ix-iy)) g=bz(l+iz)+bz(l+iz-iy)+dy*(bz(l+iz+iy)-bz(l+iz-iy))+g+dx* & (bz(l+iz+ix)+bz(l+iz+ix-iy)+dy*(bz(l+iz+ix+iy)-bz(l+iz+ix-iy))-g) bz0=(f+dz*(g-f))*(.125*qm/c)	
C	-----	
CC	write(*,'(6f11.8)')ex0,ey0,ez0,bx0,by0,bz0	
C	<i>First half electric acceleration:</i> u0=u(n)+ex0 v0=v(n)+ey0 w0=w(n)+ez0	
C	<i>First half magnetic rotation:</i> g=2./(1.+bx0*bx0+by0*by0+bz0*bz0) ul=(u0+v0*bz0-w0*by0)*g vl=(v0+w0*bx0-u0*bz0)*g wl=(w0+u0*by0-v0*bx0)*g	
C	<i>Second half mag. rot'n & el. acc'n, and position advance:</i> u(n)=u0+vl*bz0-wl*by0+ex0 x(n)=x(n)+u(n) v(n)=v0+wl*bx0-ul*bz0+ey0 y(n)=y(n)+v(n) w(n)=w0+ul*by0-vl*bx0+ez0	
1	z(n)=z(n)+w(n) return end	
C	----- subroutine usplit (x,y,z,u,v,w) if (ifix(x).ne.ifix(x-u)) go to 1	

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	call vsplit(x,y,z,u,v,w) return	
1	ul=x-.5*(1+ifix(x)+ifix(x-u)) vl=v*(ul/u) wl=w*(ul/u) call vsplit(x,y,z,ul,vl,wl) call vsplit(x-ul,y-vl,z-wl,u-ul,v-vl,w-wl) return end	
C	----- subroutine vsplit (x,y,z,u,v,w) if (ifix(y).ne.ifix(y-v)) go to 1 call wsplit(x,y,z,u,v,w) return	
1	vl=y-.5*(1+ifix(y)+ifix(y-v)) ul=u*(vl/v) wl=w*(vl/v) call wsplit(x,y,z,ul,vl,wl) call wsplit(x-ul,y-vl,z-wl,u-ul,v-vl,w-wl) return end	
C	-----	
	subroutine wsplit (x,y,z,u,v,w) if (ifix(z).ne.ifix(z-w)) go to 1 call depsit(x,y,z,u,v,w) return	
1	wl=z-.5*(1+ifix(z)+ifix(z-w)) ul=u*(wl/w) vl=v*(wl/w) call depsit(x,y,z,ul,vl,wl) call depsit(x-ul,y-vl,z-wl,u-ul,v-vl,w-wl) return end	
C	-----	
	subroutine depsit (x,y,z,u,v,w) common /fields/ ex(8192),ey(8192),ez(8192), &bx(8192),by(8192),bz(8192) dimension sm(30),ms(30) equivalence (ez(8002),q),(ez(8003),sm(1)), &(ez(8033),ms(1)),(ms(28),ix),(ms(29),iy),(ms(30),iz)	
C	<i>cell indices of half-way point:</i> i=x-.5*u j=y-.5*v k=z-.5*w	
C	<i>displacements in cell of half-way point:</i> dx=x-.5*u-i dy=y-.5*v-j dz=z-.5*w-k i=i+iy*(j-1)+iz*(k-1)	
C	<i>current elements:</i> qu=q*u qv=q*v qw=q*w delt=.083333333*qu*v*w	
C	<i>Directive specifically for the CRAY cft77 compiler:</i> cdirc\$ ivdep	
C	<i>This will make the compiler use the "gather-scatter" hardware.</i> do 1 n=1,27 ex(ms(n)+i+iy+iz)=ex(ms(n)+i+iy+iz)-sm(n)*(qu*dy*dz+delt) ex(ms(n)+i+iz)=ex(ms(n)+i+iz)-sm(n)*(qu*(1.-dy)*dz-delt) ex(ms(n)+i+iy)=ex(ms(n)+i+iy)-sm(n)*(qu*dy*(1.-dz)-delt) ex(ms(n)+i)=ex(ms(n)+i)-sm(n)*(qu*(1.-dy)*(1.-dz)+delt) ey(ms(n)+i+iz+ix)=ey(ms(n)+i+iz+ix)-sm(n)*(qv*dz*dx+delt) ey(ms(n)+i+ix)=ey(ms(n)+i+ix)-sm(n)*(qv*(1.-dz)*dx-delt) ey(ms(n)+i+iz)=ey(ms(n)+i+iz)-sm(n)*(qv*dz*(1.-dx)-delt) ey(ms(n)+i)=ey(ms(n)+i)-sm(n)*(qv*(1.-dz)*(1.-dx)+delt) ez(ms(n)+i+ix+iy)=ez(ms(n)+i+ix+iy)-sm(n)*(qw*dx*dy+delt) ez(ms(n)+i+iy)=ez(ms(n)+i+iy)-sm(n)*(qw*(1.-dx)*dy-delt) ez(ms(n)+i+ix)=ez(ms(n)+i+ix)-sm(n)*(qw*dx*(1.-dy)-delt)	

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1  ez(ms(n)+i)=ez(ms(n)+i)-sm(n)*(qw*(1.-dx)*(1.-dy)+delt)
   return
   end
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