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1  /* delaunay3 Delaunay/Power diagrams in 3d Jack Snoeyink Aug 2003
2  Implements Watson's incremental Delaunay, with sphere-based search and
3  simplical data structure storing vertices and opposite neighbors.
4  Points must be scaled to integers; guaranteed for differences of 10
5  bits, and uses leveling and hilbert curve to guarantee 16 bits if the
6  points are well distributed. Works for pdb files, which are 20 bits.
7  Handles degeneracies by perturbing points by increasing infinitesimals
8  to guarantee that all simplices are full-dimensional.
9  */
10
11 #ifndef DELAUNAY3_H
12 #define DELAUNAY3_H
13
14 #include <math.h>
15 #include <stdio.h>
16 #include <stdlib.h>
17 #include <string.h>
18
19 typedef float coord; // We'll just use floats for x,y,z coordinates
20
21 typedef struct { // Basic point data structure element
22     int index; // index back to original line in file.
23     coord x,y,z; double sq; // coordinates: 3 spatial + lifted
24 } pointType, *ppointType;
25
26 //tetrahedra are groups of four consecutive corners
27 typedef struct cornerType { // data associated with each corner
28     ppointType v; // index of vertex
29     int opp; // pointer to opposite corner in neighboring tetra
30 } cornerType, *pcornerType;
31
32 /* Tetrahedra are groups of four corners in order of increasing
33 vertex index, except that the first two may be swapped to ensure
34 that the orientation determinant is positive.
35 I.e., take the lex smallest alternating permutation with positive sign.
36 There must always be an odd number of swaps between two permutations;
37 we swap the first two if necessary to achieve this. */
38
39 /* d3.c Delaunay/Power diagram function
40 d3batch takes input vertices, and returns a (compact) corner table for Delaunay.
41 REQUIRES that the first point is at infinity,
42 and that the first 5 are in general position.
43 (I should probably verify or relax this.)
44 Since all points have radii assigned already, it can handle power diagrams.
45 */
46 void d3batch(ppointType vert, int nvert, // input vertices (pointType[]) & number of vertices
47     pcornerType *result, int *ncorners); // output corner table
48
49
50 #define XX 0
51 #define YY 1
52 #define ZZ 2
53
54 #define NVERT 5000 // number of random vertices
55 #define MAXVERT 200000 // pdb has 5 digit atom# field
56 #define TETperV 10 //
57 #define FORGETLIMIT 10000 // forget tetra after this many (for better locality of ref? Doesn't help.)
58
59 // Some useful definitions
60 #define EQUALV(i,j) (vert[i].x == vert[j].x && vert[i].y == vert[j].y && vert[i].z == vert[j].z)
61 #define EQUALPV(pv,v) (pv->x == v->x && pv->y == v->y && pv->z == v->z)
62
63 #define DET2(p,q,i,j) ((i##p)*(j##q) - (j##p)*(i##q))
64 #define DOT(a,b) ((a)->x*(b)->x + (a)->y*(b)->y + (a)->z*(b)->z)
65
66 // Stack data structure operations
67 #define STACKMAX 2000
68 #define POP(stack) (stack##st[stack##sp--])
69 #define isEmpty(stack) (stack##sp < 0)
70 #define stkINIT(stack) {stack##sp = -1; }
71
72 #ifndef STATS
73 #define PUSH(value, stack) { stack##st[++stack##sp] = value; }
74 #define stkDECLARE(stack,stn) int stack##sp, stack##st[STACKMAX];
75 #else
76 #define PUSH(value, stack) { \
77     stack##st[++stack##sp] = value; \
78     if (stack##max < stack##sp) { stack##max = stack##sp; \
79     if (stack##max >= STACKMAX) { \
80         printf("ERROR: overflow stack %x pushing %d", stack##st, value); exit(EXIT_FAILURE); } } /**\
81     }
82 #define stkDECLARE(stack,stn) int stack##sp, stack##st[STACKMAX]; int stack##max; //AUDIT /**/
83 #endif
84
85 typedef struct sphereType { // sphere equation
86     double x, y, z, sq; // Invariant sq > 0 for all created tetra, unless they use pt at infity
87 } sphereType, *psphereType;
88
89 typedef struct {
90     ppointType vert; // vertices: 0th is point at infinity!!!
91     pcornerType s; // corner table
92     psphereType sph; // spheres
93     int *active; // which spheres are active
94     int freeTetra; // head for free list for tetrahedra kept in opp[CORNER(tetra,0)]
95     int liveTetra; // latest tetra; known to be live.

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96  int maxTetra; // AUDIT only
97  int limitmaxTetra; // limit on # of created tetrahedra, spheres & corners/4.
98  // stacks used in inserting pv
99  stkDECLARE(dfs, "dfs"); // DFS stack to find dead tetras
100 stkDECLARE(idfs, "idfs"); // DFS stack for tetras adj to infinite vertex (>4*30)
101 stkDECLARE(nhbr, "nhbr"); // stack for dead corners with live neighbors
102 stkDECLARE(kill, "kill"); // stack for base corners of tetras to recycle
103 } d3stateType, *pd3stateType;
104
105 // readers call setVert when they make a point
106 void setVert(ppointType v, int indx, double xx, double yy, double zz,
107             double rad, double mult);
108
109 #define VSUBASSN(vin, xx,yy,zz, vout) {\
110     vout->index = vin->index; vout->sq = vin->sq;\
111     vout->x = vin->x - xx; vout->y = vin->y - yy; vout->z = vin->z - zz;\
112 }
113
114 //Some compiler/unix variants
115 #ifndef FALSE
116 #define FALSE 0
117 #endif
118
119 #ifndef TRUE
120 #define TRUE 1
121 #endif
122
123 #ifndef strcasecmp
124 #define strcasecmp(s1,s2)      strcmp(s1,s2)
125 #define strncasecmp(s1,s2,n)  strncmp(s1,s2,n)
126 #endif
127
128 #define HIGHCOORD 0x4000
129 #define COORDMASK 0x3fff
130
131 #ifdef bcc
132 #define RANDBIT (random(2)) // one random bit
133 #define RAND2BIT (random(4)) // two random bits
134 #define RANDPROB(mask) (random(mask+1)) // random bits masked
135 #define RANDCOORD (double)random(HIGHCOORD);
136 #define RANDOM(k) random(k) // random number 0..k-1
137 #else
138 #define RANDBIT (random()&1) // one random bit
139 #define RAND2BIT (random()&3) // two random bits
140 #define RANDPROB(mask) (mask&random()) // random bits masked
141 #define RANDCOORD (double)(random()&COORDMASK)
142 #define RANDOM(k) random()%(k) // random number 0..k-1
143 #endif
144
145 // fprintf(stderr, "\nASSERT FAILED (line %d of %s ): %s\n",
146 #ifndef NOASSERT
147 #define ASSERT(bool, string) if (!(bool)) {\
148     printf("\nASSERT FAILED (line %d of %s ): %s\n", \
149         __LINE__, __FILE__, string); }
150 #else
151 #define ASSERT(bool, string)
152 #endif
153
154 #endif
155

```

```

1  /* d3 Delaunay triangulator in 3d Jack Snoeyink Aug 2003
2  Implements Watson's incremental Delaunay, with sphere-based search and
3  simplical data structure storing vertices and opposite neighbors.
4  Handles degeneracies by perturbing points by increasing infinitesimals.
5  Guaranteed for integer coordinates of 10 bits. No flat simplices.
6  */
7
8  #include <math.h>
9
10 /* d3.c Delaunay/Power diagram function
11 d3batch takes input vertices, and returns a (compact) corner table for Delaunay.
12 REQUIRES that the first point is at infinity,
13 and that the first 5 are in general position. (I should verify or relax this.)
14 Since all points have radii assigned already, it can produce power diagrams.
15 */
16 void d3batch(ppointType vert, int nvert, // input vertices (pointType[]) & number of vertices
17 pcornerType *result, int *ncorners); // output corner table
18
19 /* void d3initialize(const pd3stateType this, ppointType vertArray, int nvert)
20 initialize d3state this from vertArray. Allocates memory for corners and spheres,
21 sets up the free list for tetrahedra, and creates spheres for the first five points.
22 REQUIRES: vertArray[0] contains the point at infinity and vertArray[1..4] contain
23 four finite points; these first five points must be in general position.
24 */
25 void d3initialize(const pd3stateType this, ppointType vertArray, int nvert);
26
27 // LOCATION ROUTINES walk a mesh stored in s, active, & sph starting from corner start to find a point pv.
28 // result is the index of a simplex whose sphere strictly contains pv.
29 // (The simplex itself need not contain pv.)
30 // The return code is positive if we succeed (# of location steps at present)
31 // Return code of 0 means that we failed, perhaps because points with small weight have no Voronoi cells
32 // Return code of -1 means that we found the duplicate of a vertex in the mesh. IN THIS CASE, result
33 // is the location of the corner where we found the duplicate!
34 int d3locSphere(const pd3stateType this, ppointType pv, int start,
35 int *result); // output
36
37 /* d3insert(const pd3stateType this, int vi, int p)
38 inserts the point this->vert[vi] that is contained in sphere p
39 into the delaunay triangulation stored in this.
40 (d3locSphere may be used to obtain p.)
41 */
42 void d3insert(const pd3stateType this, int vi, int p);
43
44 /* d3compactCorners(const pd3stateType this, pcornerType *result, int *ncorners);
45 Takes corner table this->s in which some corners/tetrahedra are unused, and
46 returns a compactified corner table result, and its length ncorners.
47 DESTROYS the corner table s and active flags in the process.
48 */
49 int d3compactCorners(const pd3stateType this, // arrays this->s & this->active are DESTROYED!
50 pcornerType *result, int *ncorners); // output
51
52 // Functions to access corner tables
53 #define MOD4(a) (a & 3)
54 #define TETRA(corner) ((corner) >> 2)
55 #define INDEX(corner) (MOD4(corner))
56 #define CORNER(tetra, index) (((tetra) << 2) + (index))
57 #define BASECORNER(corner) ((corner) & 0xFFFFFFF)
58 #define LASTCORNER(corner) ((corner) | 3)
59
60 #define DEAD(p) (this->active[p] <= 0) // is this a dead or killed tetrahedron?
61 #define KILL(p) {this->active[p] = -1;} // kill tetrahedron
62 // #define DEAD(p) (sph[p].sq < 0) // is this a dead tetrahedron?
63 // #define KILL(p) {sph[p].sq = -1;} // kill tetrahedron
64
65 #define infiniteV(pv, vert) ((pv) == vert) // first point is at infinity
66 #define infiniteC(c) infiniteV(this->s[c].v, this->vert) // corner uses inf pt
67 #define infiniteP(p) (this->sph[p].sq == 0.0) // if tetra uses infinite point
68
69 /* Tetrahedra are groups of four corners in order of increasing
70 vertex index, except that the first two may be swapped to ensure
71 that the orientation determinant is positive.
72 I.e., take the lex smallest alternating permutation with positive sign.
73 There must always be an odd number of swaps between two permutations;
74 we swap the first two if necessary to achieve this.
75 */
76
77 // set corner's vertex and opposite in tetrahedron structure
78 // void setCornerVC(int c, int vv, int op) {
79 #define setCornerVC(c, vv, op) { this->s[c].v = vv; this->s[c].opp = op; }
80 #define setCornerPairV(c, op, vv, ov) { setCornerVC(c, vv, op); setCornerVC(op, ov, c); }
81 #define setCornerVCN(c, vv, op) { setCornerVC(c, vv, op); this->s[op].opp = c; } // set corner & adjust nhbr
82 opp

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```

1  /* d3 Delaunay triangulation in 3d      Jack Snoeyink Aug 2003
2  Implements Watson's incremental Delaunay, with sphere-based location,
3  and simplical data structure storing vertices and opposite neighbors.
4  Handles degeneracies by perturbing points by increasing infinitesimals.
5  Guaranteed for integer coordinates of 10 bits. No flat simplices.
6  */
7
8  #include "delaunay3.h"
9  #include "d3.h"
10
11
12  #define spdot(sp,pv,sv) ((sp)->x*((pv)->x-(sv)->x)+(sp)->y*((pv)->y-(sv)->y)\
13      +(sp)->z*((pv)->z-(sv)->z)+(sp)->sq*((pv)->sq-(sv)->sq))
14  #define spdotInf(sp,pv) (sp)->sq
15
16  /* Allocate or free space for a tetrahedron.
17  When allocating, this->liveTetra is the location fo the new tetrahedron.
18  */
19  #define STARTTETRA(this) \
20  { startTetraCnt++; (this)->liveTetra = (this)->freeTetra; \
21    (this)->freeTetra = (this)->s[CORNER((this)->liveTetra,0)].opp; \
22    ASSERT(DEAD((this)->liveTetra), "Reusing existing tetrahedron?"); (this)->active[(this)->liveTetra] = 1; \
23
24    if ((this)->maxTetra <= (this)->liveTetra) { (this)->maxTetra = (this)->liveTetra+1; \
25    if ((this)->liveTetra >= (this)->limitmaxTetra) { printf("AUDIT: %d > limitmaxTetra\n", (this)->liveTetra)
26    ; exit(EXIT_FAILURE); } }/**\
27  } //AUDIT
28
29  #define FREETETRA(this, p) \
30  { freeTetraCnt++; /*TESTING*/ ASSERT((this)->active[p]<0, "Freeing already free tetrahedron?"); /**\
31    (this)->active[p]=0; if (((this)->maxTetra-p)<FORGETLIMIT) {\
32    (this)->s[CORNER(p,0)].opp = (this)->freeTetra; (this)->freeTetra = p; /**/ \
33  } }
34
35  //Tetrahedron manipulation tables
36  static const short offset[4][4] = { // c+offset[i][INDEX(c)] advances c to (c+i)mod5
37    /*0*/{0,0,0,0}, /*1*/{1,1,1,-3}, /*2*/{2,2,-2,-2}, /*3*/{3,-1,-1,-1}};
38  #define INCREMENT(c) (c+offset[1][INDEX(c)])
39  // drop[i] contains new vertex order after vertex i is dropped and replaced by pv on same side.
40  // offdr[i] contains drop(i)-index(i)
41  // invdrop[i][k]=j whenever drop[i][j]=k. 4s signal i=k; bad because i is dropped.
42  static const short drop[4][3] = {{2,1,3}, {0,2,3}, {1,0,3}, {0,1,2}};
43  static const short offdr[4][3] = {{2,1,3}, {-1,1,2}, {-1,-2,1}, {-3,-2,-1}};
44  static const short invdrop[4][4] = {{4,1,0,2}, {0,4,1,2}, {1,0,4,2}, {0,1,2,4}};
45
46  #include "d3audit.c"
47
48  inline double InSpherev(psphereType sp, ppointType pv, ppointType sv) {
49    double d = spdot(sp, pv, sv); // Return true if inside (==negative)
50    inSphereCnt++; /*TESTING*/
51    return d; // perturb those on sphere to inside
52  }
53
54  inline void makeSphereV(psphereType sp, ppointType v0, ppointType v1, ppointType v2, ppointType pv, ppointType
55  pe vert) {
56    double x0, y0, z0, sq0, x1, y1, z1, sq1, x2, y2, z2, sq2;
57    double xy, xz, xs, yz, ys, zs; //2x2 minors
58    // make sphere: only v0 or v1 may be infinte.
59    sphereCnt++; /*TESTING*/
60    if(!infiniteV(v0, vert)) {
61      x0 = v0->x - pv->x; y0 = v0->y - pv->y;
62      z0 = v0->z - pv->z; sq0 = v0->sq - pv->sq;
63    } else { x0 = v0->x; y0 = v0->y; z0 = v0->z; sq0 = v0->sq; }
64    if(!infiniteV(v1, vert)) {
65      x1 = v1->x - pv->x; y1 = v1->y - pv->y;
66      z1 = v1->z - pv->z; sq1 = v1->sq - pv->sq;
67    } else { x1 = v1->x; y1 = v1->y; z1 = v1->z; sq1 = v1->sq; }
68    x2 = v2->x - pv->x; y2 = v2->y - pv->y;
69    z2 = v2->z - pv->z; sq2 = v2->sq - pv->sq;
70    xy = DET2(0,1,x,y);
71    xz = DET2(0,1,x,z);
72    yz = DET2(0,1,y,z);
73    xs = DET2(0,1,x,sq);
74    ys = DET2(0,1,y,sq);
75    zs = DET2(0,1,z,sq);
76    sp->x = -y2*zs + z2*ys -sq2*yz;
77    sp->y = x2*zs - z2*xs +sq2*xz;
78    sp->z = -x2*ys + y2*xs -sq2*xy;
79    sp->sq = x2*yz - y2*xz + z2*xy;
80    // sp->w = -p2->x*sp->x -p2->y*sp->y -p2->z*sp->z -p2->sq*sp->sq;
81    /* printf("disp('Sphere equation: <%5.0f %5.0f %5.0f %5.0f %5.0f>'\n",sp->x,sp->y,sp->z,sp->sq);
82    (void)fflush(stdout);
83    printf("%%Sp ck: %g %g %g %g\n", spdot(sp,v0), spdot(sp,v1), spdot(sp,v2), spdot(sp,pv)); */

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84 // when we initialize, this is what we fill in.
85 //const int initialopp[] = {11,5,15,21,25, 1,10,16,20,26, 6,0,17,22,27, 2,7,12,23,28, 8,3,13,18,29, 4,9,14,1
86 9,24};
87 static const int initialopp[5][4] = {
88     {CORNER(1,1), CORNER(2,0), CORNER(3,1), CORNER(4,0)},
89     {CORNER(2,1), CORNER(0,0), CORNER(3,0), CORNER(4,1)},
90     {CORNER(0,1), CORNER(1,0), CORNER(3,2), CORNER(4,2)},
91     {CORNER(1,2), CORNER(0,2), CORNER(2,2), CORNER(4,3)},
92     {CORNER(0,3), CORNER(1,3), CORNER(2,3), CORNER(3,3)};
93
94 static const int initialv[2][5][4] = {{{{1,2,3,4}, {2,0,3,4}, {0,1,3,4}, {1,0,2,4}, {0,1,2,3}},
95                                         {{0,2,3,4}, {2,1,3,4}, {1,0,3,4}, {0,1,2,4}, {1,0,2,3}}}};
96
97
98 /* void d3initialize(const pd3stateType this, ppointType vertArray, int nvert)
99 initialize d3state this from vertArray. Allocates memory for corners and spheres,
100 sets up the free list for tetrahedra, and creates spheres for the first five points.
101 REQUIRES: vertArray[0] contains the point at infinity and vertArray[1..4] contain
102 four finite points; these first five points must be in general position.
103 */
104 void d3initialize(const pd3stateType this, ppointType vertArray, int nvert) {
105     int j, p, last;
106     double d;
107
108     // initBitTable(); // BITS
109     this->vert = vertArray;
110     this->limitmaxTetra = TETperV*nvert; // allocate space for spheres and corners
111     this->s = (pcornerType) calloc(4*this->limitmaxTetra, sizeof(cornerType)); // per corner: v, opp
112     this->sph = (psphereType) calloc(this->limitmaxTetra, sizeof(sphereType)); // per tetra: sphere eqn
113     this->active = (int *) calloc(this->limitmaxTetra, sizeof(int)); // flag -1 unused, 0 dead, 1 alive
114
115     if ((this->s == NULL) || (this->sph == NULL) || (this->active == NULL)) {
116         printf("ERROR: d3batch could not calloc memory for data structures\n");
117         exit(EXIT_FAILURE);
118     }
119
120     // initialize tetrahedra
121     last = -1; /* set up free list of tetrahedra */
122     this->freeTetra = this->limitmaxTetra;
123     do {
124         this->freeTetra--;
125         this->active[this->freeTetra] = 0; // KILL(freeTetra);
126         this->s[CORNER(this->freeTetra,0)].opp = last;
127         last = this->freeTetra;
128     } while (this->freeTetra > 5);
129
130     this->active[4] = 2; // create first sphere
131     makeSphereV(this->sph+4, this->vert+0, this->vert+1, this->vert+2, this->vert+3, this->vert);
132     d = spdot(this->sph+4, this->vert+4, this->vert+3); // if d<0, then we need to swap
133
134     if (d == 0.0) {
135         printf("ERROR: Need first five vertices to be in general position"); exit(EXIT_FAILURE);
136     }
137
138     if (d < 0) {
139         this->sph[4].x = -this->sph[4].x; this->sph[4].y = -this->sph[4].y; this->sph[4].z = -this->sph[4].z;
140         this->sph[4].sq = -this->sph[4].sq;
141     }
142
143     for (p=0; p<5; p++) {
144         for (j=0; j<4; j++) { // pay attention to orientation when assigning vertices
145             setCornerVC(CORNER(p,j), this->vert+initialv[d<0][p][j], initialopp[p][j]);
146         }
147         makeSphereV(this->sph+p, this->s[CORNER(p,0)].v, this->s[CORNER(p,1)].v, this->s[CORNER(p,2)].v, this->s
[CORNER(p,3)].v, this->vert);
148         this->active[p] = 1;
149         // swap first two if d<0.
150         if (((d<0)&&(p==1)) || ((d>0) && (p==0)))
151             {ASSERT(this->sph[p].sq > 0, "Somehow vertp at infinity is in or on sphere p in init");}
152         else
153             {ASSERT(spdot(this->sph+p, this->vert+p + (d<0)*(p<2)*(1-2*p), this->s[CORNER(p,3)].v) > 0,
154                     "Somehow vertp is in or on sphere p in init.");}
155     }
156     this->liveTetra = 4;
157     this->maxTetra = 5;
158 }
159
160
161

```

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```

162 // LOCATION ROUTINES walk a mesh stored in s, active, & sph starting from corner start to find a point pv.
163 // result is the index of a simplex whose sphere strictly contains pv.
164 // (The simplex itself need not contain pv.)
165 // The return code is positive if we succeed (# of location steps at present)
166 // Return code of 0 means that we failed, perhaps because points with small weight have no Voronoi cells
167 // Return code of -1 means that we found the duplicate of a vertex in the mesh. IN THIS CASE, result
168 // is the location of the corner where we found the duplicate!
169 int d3locSphere(const pd3stateType this, ppointType pv, int start,
170               int *result) { // output
171     int j, guard; // loop variables
172     int c1, c2; // corners
173     psphereType s1, s2; // spheres
174     double I1, I2, d; // InSphere values
175
176     guard = 2*this->maxTetra+4; // prevent infinite loops
177     c1 = CORNER(start, 0); // corner in start
178     s1 = this->sph+start; // sphere at start
179     I1 = InSphereV(s1, pv, this->s[c1+3].v); // Check if inside start sphere.
180     if ( (I1 < 0) || (I1 == 0 && s1->sq > 0) ) { // found already
181         *result = start;
182         return 1; // success on first try
183     }
184
185     while (--guard) {
186         c2 = this->s[c1].opp; s2 = this->sph + TETRA(c2); // nhbr corner, sphere, value
187         I2 = InSphereV(s2, pv, this->s[LASTCORNER(c2)].v);
188         if ( (I2 < 0) || (I2 == 0 && s2->sq > 0) ) { // found one!
189             *result = s2 - this->sph;
190             return 2*this->maxTetra+5-guard; // number of steps
191         }
192         d = s2->sq * I1 - s1->sq * I2; // Warning: if s1 & s2 are same sphere, this is zero
193         locateSideCnt++; // STATS
194         if (d==0) { // We are on a sphere---check for duplicate vertex
195             if (EQUALPV(pv, this->s[c2].v)) { *result = c2; return -1; }
196             j = INDEX(c2);
197             if (EQUALPV(pv, this->s[c2+offset[1][j]].v)) { *result = c2+offset[1][j]; return -1; }
198             if (EQUALPV(pv, this->s[c2+offset[2][j]].v)) { *result = c2+offset[2][j]; return -1; }
199             if (EQUALPV(pv, this->s[c2+offset[3][j]].v)) { *result = c2+offset[3][j]; return -1; }
200             // otherwise no duplicate; we probably have s1 == s2. (Rare in protein data.)
201             d = RANDBIT-0.5; // choose a random direction, as a hack. (Should do plane computation)
202         }
203         if (d < 0) // if on I1 side
204             c1 = INCREMENT(c1);
205         else { // on I2 side
206             c1 = INCREMENT(c2); s1 = s2; I1 = I2;
207         }
208     }
209     result = 0; // location failure
210     return 0;
211 }
212
213 /* d3compactCorners(const pd3stateType this, pcornerType *result, int *ncorners);
214 Takes corner table this->s in which some corners/tetrahedra are unused, and
215 returns a compactified corner table result, and its length ncorners.
216 DESTROYS the corner table s and active flags in the process.
217 returns false if it is unable to allocate memory.
218 */
219
220 int d3compactCorners(const pd3stateType this, // arrays this->s & this->active DESTROYED!
221                    pcornerType *result, int *ncorners) { // output
222     int c, nc, i, j;
223     pcornerType pc;
224
225     i = 0; // count actives
226     for (j = 0; j < this->maxTetra; j++)
227         this->active[j] = (DEAD(j)) ? -1 : i++; // make old->new pointer dictionary for active tetra
228
229     *ncorners = 4*i; // number of corners to return
230     *result = pc = (pcornerType) calloc(*ncorners, sizeof(cornerType)); // return corner table: v, opp
231     if (pc != NULL) {
232         for (j = 0; j < this->maxTetra; j++) // compact the corners
233             if (this->active[j] >= 0) {
234                 c = CORNER(j, 0); // old corner c --> new corner ptr pc = (*result)+0,1,2,...
235                 pc->v = this->s[c].v; nc = this->s[c].opp;
236                 pc->opp = CORNER(this->active[TETRA(nc)], INDEX(nc)); // assign new tetra # w/ old index
237                 pc++; c++;
238                 pc->v = this->s[c].v; nc = this->s[c].opp;
239                 pc->opp = CORNER(this->active[TETRA(nc)], INDEX(nc));
240                 pc++; c++;
241                 pc->v = this->s[c].v; nc = this->s[c].opp;
242                 pc->opp = CORNER(this->active[TETRA(nc)], INDEX(nc));
243                 pc++; c++;
244                 pc->v = this->s[c].v; nc = this->s[c].opp;
245                 pc->opp = CORNER(this->active[TETRA(nc)], INDEX(nc));
246                 pc++;
247             }
248     }
249     free(this->s); // free old corner list
250     free(this->active);
251     return (pc != NULL); // true if we were successful
252 }
253
254
255

```

```

256
257 /* d3insert(const pd3stateType this, int vi, int p)
258 inserts the point this->vert[vi] that is contained in sphere p
259 into the delaunay triangulation stored in this.
260 (d3locSphere may be used to obtain p.)
261 */
262 void d3insert(const pd3stateType this, int vi, int p) {
263     int i, j, off;
264     int b, c, newb; // corners
265     int nc, ni, dead, jdead; // indices
266     double d;
267     ppointType v0, v1, v2; // pointers to vertices
268     ppointType pv = this->vert+vi;
269
270     // Tetrahedra containing pv are "dead", and are pushed onto kill stack.
271     // We use DFS with stack pst to find them and kill them
272     // At live-dead boundary, we save dead tetras on stack nhbr,
273     // then make new tetras and hook in to live by setting the last opp pointer.
274     //
275     // Invariants/operations: Tetrahedron p is marked alive or dead on first visit.
276     // Corner c is pushed on stack when TETRA(this->s[c].opp) is marked dead.
277     //
278     // On termination, stack nhbr contains dead corners with live neighbors
279     // that have new tetras (so this->s[nhbr].opp != this->s[this->s[nhbr].opp].opp temporarily.)
280     // Stack kill contains old tetrahedra for final recycling.
281
282     stkINIT(this->dfs); // DFS stack holds corners opposite dead tetras
283     stkINIT(this->idfs); // iDFS stack holds corners opposite infinite tetras with pv on bdry
284     // (these are a special case: dead, but don't propagate)
285     stkINIT(this->nhbr); // stack for dead corners with live nhbr tetras
286     stkINIT(this->kill); // stack of dead tetras to recycle
287     b = CORNER(p, 0);
288     PUSH(p, this->kill); KILL(p); // kill tetra initial p,
289     PUSH(this->s[b++].opp, this->dfs); // stack neighbors
290     PUSH(this->s[b++].opp, this->dfs);
291     PUSH(this->s[b++].opp, this->dfs);
292     PUSH(this->s[b ].opp, this->dfs);
293
294     while (!isEmpty(this->dfs)) {
295         c = POP(this->dfs); p = TETRA(c);
296         /* printf("Popping %d with opp %d\n", c, this->s[c].opp); */
297         ASSERT(DEAD(TETRA(this->s[c].opp)), "dfs stack element with non-dead neighbor");
298         if (DEAD(p)) continue; // dead already
299         d = InSpherev(this->sph + p, pv, this->s[LASTCORNER(c)].v); // Is pv in, out, or on?
300         if (d < 0) { // kill and continue dfs if pv is strictly inside
301             KILL(p); PUSH(p, this->kill); // kill and stack tetra
302             j = INDEX(c);
303             PUSH(this->s[c+offset[1][j]].opp, this->dfs); // stack neighbors to check
304             PUSH(this->s[c+offset[2][j]].opp, this->dfs);
305             PUSH(this->s[c+offset[3][j]].opp, this->dfs);
306         }
307         else if (d > 0 || this->sph[p].sq > 0) { // pv is outside (or on with sp finite), so
308             // c is live neighbor of dead opp tetra this->s[c].opp
309             PUSH(this->s[c].opp, this->nhbr); // remember old corner, so we can hook tetra into mesh later
310             STARTTETRA(this); // make new tetrahedron liveTetra
311             newb = CORNER(this->liveTetra, 3); // last corner of new tetra
312             setCornerVCN(newb, pv, c); // last corner is pv; also set opposite corner c. Do rest later.
313         }
314         else { // d==0 && sph[p] is infinite: handle two special cases
315             if (this->sph[TETRA(this->s[c].opp)].sq == 0) { // if dead sphere is infinite, too
316                 PUSH(c, this->idfs); // then if c stays alive, we make tetra to it (flat, but infinite).
317             } else { // dead sphere is finite; kill c and make tetras to neighbors, if they stay alive.
318                 KILL(p); PUSH(p, this->kill); // kill and stack tetra
319                 j = INDEX(c);
320                 PUSH(this->s[c+offset[1][j]].opp, this->idfs); // stack neighbors to check
321                 PUSH(this->s[c+offset[2][j]].opp, this->idfs);
322                 PUSH(this->s[c+offset[3][j]].opp, this->idfs);
323             }
324         }
325     }
326
327     while (!isEmpty(this->idfs)) { // check the neighbors of infinite tetrahedra
328         c = POP(this->idfs); p = TETRA(c);
329         /* printf("Popping %d with opp %d\n", c, this->s[c].opp); */
330         ASSERT(DEAD(TETRA(this->s[c].opp)), "dfs stack element with non-dead neighbor");
331         if (DEAD(p)) continue; // dead already
332         ASSERT(DEAD(TETRA(this->s[c].opp)), "Live corner c should have dead neighbor");
333         PUSH(this->s[c].opp, this->nhbr); // remember old corner, so we can hook tetra into mesh later
334         STARTTETRA(this); // make new tetrahedron liveTetra
335         newb = CORNER(this->liveTetra, 3); // last corner of new tetra
336         setCornerVCN(newb, pv, c); // last corner is pv; also set opposite corner c. Do rest later.
337     }
338
339     // Now, we have stack of dead neighbors of live tetras, and we've hooked new tetras to them.
340     while (!isEmpty(this->nhbr)) {
341         dead = POP(this->nhbr); jdead = INDEX(dead); // dead tetra and index of dropped corner.
342         /* printf("--Popped %d(%d)\n", dead, jdead); */
343         ASSERT(DEAD(TETRA(dead)), "corner on nhbr stack is not dead!?");
344         newb = this->s[this->s[dead].opp].opp-3; // base of new tetra.
345
346         dead -= jdead; // just use base of dead one.
347         // new tetra has 0,1,2,3=pv;
348         // corresponding old indices before jdead is dropped:
349         // drop[j][0]...drop[j][3], (no corresp to pv)
350         j = jdead;

```

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d3locSphere	3:170
makeSphereV	1:52

```

351 i = drop[jdead][0]; // old index of new corner 0;
352 c = dead+i; // note i= INDEX(C);
353 v0 = this->s[c].v; // copy vertex v0
354 nc = this->s[c].opp; // go to neighbor
355 // In tetra opp c, find new location of j. That is new c. New j= INDEX(c.opp).
356 // To avoid index calculations, maintain i= INDEX(c), nc = this->s[c].opp, ni= INDEX(nc).
357 while (DEAD(TETRA(nc))) {
358     ni = INDEX(nc); off = indoff[i][ni][j]; // where j goes relative to i is our new i.
359     j = ni; i = ni + off; c = nc + off; nc = this->s[c].opp; // fix new j, i, c, and try neighbor
360 }
361 nc = this->s[nc].opp; // go to new tetra
362 ASSERT(this->s[nc].v == pv, "Expected to find new tetra using pv after walking dead tetras. ");
363
364 setCornerVC(newb, v0, nc-3+invdrop[i][j]); newb++;
365
366 j = jdead;
367 i = drop[jdead][1]; // old index of new corner 1;
368 c = dead+i; // note i= INDEX(C);
369 v1 = this->s[c].v; // copy vertex v1
370 nc = this->s[c].opp; // go to neighbor
371 // In tetra opp c, find new location of j. That is new c. New j= INDEX(c.opp).
372 // To avoid index calculations, maintain i= INDEX(c), nc = this->s[c].opp, ni= INDEX(nc).
373 while (DEAD(TETRA(nc))) {
374     ni = INDEX(nc); off = indoff[i][ni][j]; // where j goes relative to i is our new i.
375     j = ni; i = ni + off; c = nc + off; nc = this->s[c].opp; // fix new j, i, c, and try neighbor
376 }
377 nc = this->s[nc].opp; // go to new tetra
378 ASSERT(this->s[nc].v == pv, "Expected to find new tetra using pv after walking dead tetras. ");
379
380 setCornerVC(newb, v1, nc-3+invdrop[i][j]); newb++;
381
382 j = jdead;
383 i = drop[jdead][2]; // old index of new corner 2;
384 c = dead+i; // note i= INDEX(C);
385 v2 = this->s[c].v; // copy vertex v2
386 nc = this->s[c].opp; // go to neighbor
387 // In tetra opp c, find new location of j. That is new c. New j= INDEX(c.opp).
388 // To avoid index calculations, maintain i= INDEX(c), nc = this->s[c].opp, ni= INDEX(nc).
389 while (DEAD(TETRA(nc))) {
390     ni = INDEX(nc); off = indoff[i][ni][j]; // where j goes relative to i is our new i.
391     j = ni; i = ni + off; c = nc + off; nc = this->s[c].opp; // fix new j, i, c, and try neighbor
392 }
393 nc = this->s[nc].opp; // go to new tetra
394 ASSERT(this->s[nc].v == pv, "Expected to find new tetra using pv after walking dead tetras. ");
395
396 setCornerVC(newb, v2, nc-3+invdrop[i][j]); newb++;
397
398 c = this->s[this->s[dead+jdead].opp].opp;
399 ASSERT(v0==this->s[CORNERINOPP(0,c)].v, "v0 does not line up");
400 ASSERT(v1==this->s[CORNERINOPP(1,c)].v, "v1 does not line up");
401 ASSERT(v2==this->s[CORNERINOPP(2,c)].v, "v2 does not line up");
402
403 makeSphereV(this->sph+TETRA(newb), v0, v1, v2, pv, this->vert); // use either this or makeSphereP abov
404 e
405 }
406
407
408

```

Functions

InSphereV	1:46
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410	<i>InSphereV</i> 1:46
411	<i>d3batch</i> 6:416
412	<i>d3compactCorners</i> 3:220
413	<i>d3initialize</i> 2:104
414	<i>d3insert</i> 4:262
415	<i>d3locSphere</i> 3:170
416	<i>makeSphereV</i> 1:52
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```

3 */
4
5 #include <time.h>
6 #include "delaunay3.h"
7 #include "pdbreader.h"
8
9 int main(int argc, char** argv) {
10     int i, j, ii, jj;
11     int hashtb[HIGHCOORD];
12     int nexttb[NVERT];
13     ppointType vert,v;
14     int nvert, nv;
15     pcornerType result;
16     int nresult;
17
18     clock_t tic, toc;
19
20     FILE *fid;
21
22     /* fid = mdopener("none", argc, argv);
23     d3permute(fid, mdreader, &vert, &nvert);
24     fclose(fid); */
25
26     /* fid = txtopener("hilb6.txt", argc, argv);
27     d3permute(fid, txt3reader, &vert, &nvert);
28     fclose(fid); */
29
30     ii = 1;
31     for (ii = 1; ii < argc; ii++)
32         if (argv[ii][0] != '-') {
33             fid = pdbopener(argv[ii], argc < 4 ? argc : 4, argv);
34             d3permute(fid, pdbreader, &v, &nv);
35             fclose(fid);
36             tic = clock(); // start timer
37             jj = 1;
38 #ifndef NOASSERT
39             for (jj = 0; jj < 10; jj++)
40 #endif
41                 {
42                     d3batch(v, nv, &result, &nresult);
43                     free(result);
44                 }
45             toc = clock();
46             printf("%s %d %d Time(secs) %f\n\n", argv[ii], nv, nresult,
47                 ((double) (toc - tic)) / CLOCKS_PER_SEC / jj); (void)fflush(stdout); /**/
48         }
49     return EXIT_SUCCESS;
50 }
51

```