**1 Introduction**

**2 Bioinformatics – Genome Similarity Using Frequency Vectors**

**2.1 Analysis**

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**6.1 Original Code**

The original code for the Bioinformatics – Genome similarity using Frequency Vectors (C++) application was provided by Dr Wayne Kelly on the CAB401 High Performance and Parallel Computing QUT Blackboard page. A copy of the original code can be seen below. All bacteria files and the Visual Studio 2017 project can be found at the link here <https://github.com/Starwolf-001/CAB401/tree/master/Bioinformatics_c_assignment>.

1 #include <stdio.h>

2 #include <string.h>

3 #include <time.h>

4 #include <math.h>

5 #include <iostream>

6

7 int number\_bacteria;

8 char\*\* bacteria\_name;

9 long M, M1, M2;

10 short code[27] = { 0, 2, 1, 2, 3, 4, 5, 6, 7, -1, 8, 9, 10, 11, -1, 12, 11 13, 14, 15, 16, 1, 17, 18, 5, 19, 3 };

12 #define encode(ch) code[ch-'A']

13 #define LEN 6

14 #define AA\_NUMBER 20

15 #define EPSILON 1e-010

16

17 void Init()

18 {

19 M2 = 1;

20 for (int i = 0; i<LEN - 2; i++) // M2 = AA\_NUMBER ^ (LEN-2);

21 M2 \*= AA\_NUMBER;

22 M1 = M2 \* AA\_NUMBER; // M1 = AA\_NUMBER ^ (LEN-1);

23 M = M1 \*AA\_NUMBER; // M = AA\_NUMBER ^ (LEN);

24 }

25

26 class Bacteria

27 {

28 private:

29 long\* vector;

30 long\* second;

31 long one\_l[AA\_NUMBER];

32 long indexs;

33 long total;

34 long total\_l;

35 long complement;

36

37 void InitVectors()

38 {

39 vector = new long[M];

40 second = new long[M1];

41 memset(vector, 0, M \* sizeof(long));

42 memset(second, 0, M1 \* sizeof(long));

43 memset(one\_l, 0, AA\_NUMBER \* sizeof(long));

44 total = 0;

45 total\_l = 0;

46 complement = 0;

47 }

48

49 void init\_buffer(char\* buffer)

50 {

51 complement++;

52 indexs = 0;

53 for (int i = 0; i<LEN - 1; i++)

54 {

55 short enc = encode(buffer[i]);

56 one\_l[enc]++;

57 total\_l++;

58 indexs = indexs \* AA\_NUMBER + enc;

59 }

60 second[indexs]++;

61 }

62

63 void cont\_buffer(char ch)

64 {

65 short enc = encode(ch);

66 one\_l[enc]++;

67 total\_l++;

68 long index = indexs \* AA\_NUMBER + enc;

69 vector[index]++;

70 total++;

71 indexs = (indexs % M2) \* AA\_NUMBER + enc;

72 second[indexs]++;

73 }

74

75 public:

76 long count;

77 double\* tv;

78 long \*ti;

79

80 Bacteria(char\* filename)

81 {

82 FILE \* bacteria\_file = fopen(filename, "r");

83 InitVectors();

84

85 char ch;

86 while ((ch = fgetc(bacteria\_file)) != EOF)

87 {

88 if (ch == '>')

89 {

90 // skip rest of line

91 while (fgetc(bacteria\_file) != '\n');

92 char buffer[LEN - 1];

93 fread(buffer, sizeof(char), LEN - 1, bacteria\_file);

94 init\_buffer(buffer);

95 }

96 else if (ch != '\n')

97 cont\_buffer(ch);

98 }

99

100 long total\_plus\_complement = total + complement;

101 double total\_div\_2 = total \* 0.5;

102 int i\_mod\_aa\_number = 0;

103 int i\_div\_aa\_number = 0;

104 long i\_mod\_M1 = 0;

105 long i\_div\_M1 = 0;

106

107 double one\_l\_div\_total[AA\_NUMBER];

108 for (int i = 0; i<AA\_NUMBER; i++)

109 one\_l\_div\_total[i] = (double)one\_l[i] / total\_l;

110

111 double\* second\_div\_total = new double[M1];

112 for (int i = 0; i<M1; i++)

113 second\_div\_total[i] = (double)second[i] / total\_plus\_complement;

114 count = 0;

115 double\* t = new double[M];

116

117 for (long i = 0; i<M; i++)

118 {

119 double p1 = second\_div\_total[i\_div\_aa\_number];

120 double p2 = one\_l\_div\_total[i\_mod\_aa\_number];

121 double p3 = second\_div\_total[i\_mod\_M1];

122 double p4 = one\_l\_div\_total[i\_div\_M1];

123 double stochastic = (p1 \* p2 + p3 \* p4) \* total\_div\_2;

124

125 if (i\_mod\_aa\_number == AA\_NUMBER - 1)

126 {

127 i\_mod\_aa\_number = 0;

128 i\_div\_aa\_number++;

129 }

130 else

131 i\_mod\_aa\_number++;

132

133 if (i\_mod\_M1 == M1 - 1)

134 {

135 i\_mod\_M1 = 0;

136 i\_div\_M1++;

137 }

138 else

139 i\_mod\_M1++;

140

141 if (stochastic > EPSILON)

142 {

143 t[i] = (vector[i] - stochastic) / stochastic;

144 count++;

145 }

146 else

147 t[i] = 0;

148 }

149

150 delete second\_div\_total;

151 delete vector;

152 delete second;

153

154 tv = new double[count];

155 ti = new long[count];

156

157 int pos = 0;

158 for (long i = 0; i<M; i++)

159 {

160 if (t[i] != 0)

161 {

162 tv[pos] = t[i];

163 ti[pos] = i;

164 pos++;

165 }

166 }

167 delete t;

168

169 fclose(bacteria\_file);

170 }

171 };

172

173 void ReadInputFile(char\* input\_name)

174 {

175 FILE\* input\_file = fopen(input\_name, "r");

176 fscanf(input\_file, "%d", &number\_bacteria);

177 bacteria\_name = new char\*[number\_bacteria];

178

179 for (long i = 0; i<number\_bacteria; i++)

180 {

181 bacteria\_name[i] = new char[20];

182 fscanf(input\_file, "%s", bacteria\_name[i]);

183 strcat(bacteria\_name[i], ".faa");

184 }

185 fclose(input\_file);

186 }

187

188 double CompareBacteria(Bacteria\* b1, Bacteria\* b2)

189 {

190 double correlation = 0;

191 double vector\_len1 = 0;

192 double vector\_len2 = 0;

193 long p1 = 0;

194 long p2 = 0;

195 while (p1 < b1->count && p2 < b2->count)

196 {

197 long n1 = b1->ti[p1];

198 long n2 = b2->ti[p2];

199 if (n1 < n2)

200 {

201 double t1 = b1->tv[p1];

202 vector\_len1 += (t1 \* t1);

203 p1++;

204 }

205 else if (n2 < n1)

206 {

207 double t2 = b2->tv[p2];

208 p2++;

209 vector\_len2 += (t2 \* t2);

210 }

211 else

212 {

213 double t1 = b1->tv[p1++];

214 double t2 = b2->tv[p2++];

215 vector\_len1 += (t1 \* t1);

216 vector\_len2 += (t2 \* t2);

217 correlation += t1 \* t2;

218 }

219 }

220 while (p1 < b1->count)

221 {

222 long n1 = b1->ti[p1];

223 double t1 = b1->tv[p1++];

224 vector\_len1 += (t1 \* t1);

225 }

226 while (p2 < b2->count)

227 {

228 long n2 = b2->ti[p2];

229 double t2 = b2->tv[p2++];

230 vector\_len2 += (t2 \* t2);

231 }

232

233 return correlation / (sqrt(vector\_len1) \* sqrt(vector\_len2));

234 }

235

236 void CompareAllBacteria()

237 {

238 Bacteria\*\* b = new Bacteria\*[number\_bacteria];

239 for (int i = 0; i<number\_bacteria; i++)

240 {

241 printf("load %d of %d\n", i + 1, number\_bacteria);

242 b[i] = new Bacteria(bacteria\_name[i]);

243 }

244

245 for (int i = 0; i<number\_bacteria - 1; i++)

246 for (int j = i + 1; j<number\_bacteria; j++)

247 {

248 printf("%2d %2d -> ", i, j);

249 double correlation = CompareBacteria(b[i], b[j]);

250 printf("%.20lf\n", correlation);

251 }

252 }

253

254 int main(int argc, char \* argv[])

255 {

256 time\_t t1 = time(NULL);

257

258 Init();

259 ReadInputFile(argv[1]);

260 CompareAllBacteria();

261

262 time\_t t2 = time(NULL);

263 printf("time elapsed: %d seconds\n", t2 - t1);

264

265 system("pause");

266

267 return 0;

277 }

**6.2 High Performance and Parallel Code**

This code for the Bioinformatics – Genome similarity using Frequency Vectors (C++) application was analysed and tested to provide the correct results in a short time as per the requirement for the CAB401 High Performance and Parallel Computing Assignment. This code can be seen below. All bacteria files, notes taken during testing, code and the Visual Studio 2017 project can be found at the link here <https://github.com/Starwolf-001/CAB401/tree/master/Bioinformatics_c_assignment_high_performance>.

1 #include <stdio.h>

2 #include <string.h>

3 #include <time.h>

4 #include <math.h>

5 #include <iostream>

6 #include <omp.h>

7

8 int number\_bacteria;

9 char\*\* bacteria\_name;

10 long M, M1, M2;

11 short code[27] = {0, 2, 1, 2, 3, 4, 5, 6, 7, -1, 8, 9, 10, 11, -1, 12, 13, 14, 15, 16, 1, 17, 18, 5, 19, 3};

12 #define encode(ch) code[ch-'A']

13 #define LEN 6

14 #define AA\_NUMBER 20

15 #define EPSILON 1e-010

16

17 void Init() {

18 M2 = 1;

24 for (int i = 0; i < LEN - 2; i++) { // M2 = AA\_NUMBER ^ (LEN-2);

25 M2 \*= AA\_NUMBER;

26 }

27 M1 = M2 \* AA\_NUMBER; // M1 = AA\_NUMBER ^ (LEN-1);

28 M = M1 \*AA\_NUMBER; // M = AA\_NUMBER ^ (LEN);

29 }

30

31 class Bacteria {

32 private:

33 long\* vector;

34 long\* second;

35 long one\_l[AA\_NUMBER];

36 long indexs;

37 long total;

38 long total\_l;

39 long complement;

40

41 void InitVectors() {

42 vector = new long[M];

43 second = new long[M1];

44 memset(vector, 0, M \* sizeof(long));

45 memset(second, 0, M1 \* sizeof(long));

46 memset(one\_l, 0, AA\_NUMBER \* sizeof(long));

47 total = 0;

48 total\_l = 0;

49 complement = 0;

50 }

51

52 void init\_buffer(char\* buffer) {

53 complement++;

54 indexs = 0;

59 for (int i = 0; i < LEN - 1; i++) {

60 short enc = encode(buffer[i]);

61 one\_l[enc]++;

62 total\_l++;

63 indexs = indexs \* AA\_NUMBER + enc;

64 }

65 second[indexs]++;

66 }

67

68 void cont\_buffer(char ch) {

69 short enc = encode(ch);

70 one\_l[enc]++;

71 total\_l++;

72 long index = indexs \* AA\_NUMBER + enc;

73 vector[index]++;

74 total++;

75 indexs = (indexs % M2) \* AA\_NUMBER + enc;

76 second[indexs]++;

77 }

78

79 public:

80 long count;

81 double\* tv;

82 long \*ti;

83

84 Bacteria(char\* filename) {

92 FILE \* bacteria\_file = fopen(filename, "r");

93 InitVectors();

94

95 char ch;

96 while ((ch = fgetc(bacteria\_file)) != EOF) {

97 if (ch == '>') {

98 while (fgetc(bacteria\_file) != '\n'); // skip rest of line

99

100 char buffer[LEN - 1];

101 fread(buffer, sizeof(char), LEN - 1, bacteria\_file);

102 init\_buffer(buffer);

103 }

104 else if (ch != '\n')

105 cont\_buffer(ch);

106 }

107 fclose(bacteria\_file);

108

109 long total\_plus\_complement = total + complement;

110 double total\_div\_2 = total \* 0.5;

111 int i\_mod\_aa\_number = 0;

112 int i\_div\_aa\_number = 0;

113 long i\_mod\_M1 = 0;

114 long i\_div\_M1 = 0;

115

116 double one\_l\_div\_total[AA\_NUMBER];

117 double\* second\_div\_total = new double[M1];

130 for (int i = 0; i < AA\_NUMBER; i++) {

131 one\_l\_div\_total[i] = (double)one\_l[i] / total\_l;

132 }

138 for (int i = 0; i < M1; i++) {

139 second\_div\_total[i] = (double)second[i] / total\_plus\_complement;

140 }

141

142 count = 0;

143 double\* t = new double[M];

144

156 for (long i = 0; i < M; i++) {

157 double p1 = second\_div\_total[i\_div\_aa\_number];

158 double p2 = one\_l\_div\_total[i\_mod\_aa\_number];

159 double p3 = second\_div\_total[i\_mod\_M1];

160 double p4 = one\_l\_div\_total[i\_div\_M1];

161 double stochastic = (p1 \* p2 + p3 \* p4) \* total\_div\_2;

162

163 if (i\_mod\_aa\_number == AA\_NUMBER - 1) {

164 i\_mod\_aa\_number = 0;

165 i\_div\_aa\_number++;

166 }

167 else {

168 i\_mod\_aa\_number++;

169 }

170

171 if (i\_mod\_M1 == M1 - 1) {

172 i\_mod\_M1 = 0;

173 i\_div\_M1++;

174 }

175 else {

176 i\_mod\_M1++;

177 }

178

179 if (stochastic > EPSILON) {

180 t[i] = (vector[i] - stochastic) / stochastic;

181 count++;

182 }

183 else {

184 t[i] = 0;

185 }

186 }

187

188 delete second\_div\_total;

189 delete vector;

190 delete second;

191

192 tv = new double[count];

193 ti = new long[count];

194

195 int pos = 0;

201 for (long i = 0; i < M; i++) {

202 if (t[i] != 0) {

203 tv[pos] = t[i];

204 ti[pos] = i;

205 pos++;

206 }

207 }

208 delete t;

209 }

210 };

211

212 void ReadInputFile(char\* input\_name) {

213 FILE\* input\_file = fopen(input\_name, "r");

214 fscanf(input\_file, "%d", &number\_bacteria);

215 bacteria\_name = new char\*[number\_bacteria];

220 for (long i = 0; i < number\_bacteria; i++) {

221 bacteria\_name[i] = new char[20];

222 fscanf(input\_file, "%s", bacteria\_name[i]);

223 strcat(bacteria\_name[i], ".faa");

224 }

225 fclose(input\_file);

226 }

227

228 double CompareBacteria(Bacteria\* b1, Bacteria\* b2) {

229 double correlation = 0;

230 double vector\_len1 = 0;

231 double vector\_len2 = 0;

232 long p1 = 0;

233 long p2 = 0;

237 while (p1 < b1->count && p2 < b2->count) {

238 long n1 = b1->ti[p1];

239 long n2 = b2->ti[p2];

240 if (n1 < n2) {

241 double t1 = b1->tv[p1];

242 vector\_len1 += (t1 \* t1);

243 p1++;

244 }

245 else if (n2 < n1) {

246 double t2 = b2->tv[p2];

247 p2++;

248 vector\_len2 += (t2 \* t2);

249 }

250 else {

251 double t1 = b1->tv[p1++];

252 double t2 = b2->tv[p2++];

253 vector\_len1 += (t1 \* t1);

254 vector\_len2 += (t2 \* t2);

255 correlation += t1 \* t2;

256 }

257 }

264 while (p1 < b1->count) {

265 long n1 = b1->ti[p1];

266 double t1 = b1->tv[p1++];

267 vector\_len1 += (t1 \* t1);

268 }

274 while (p2 < b2->count) {

275 long n2 = b2->ti[p2];

276 double t2 = b2->tv[p2++];

277 vector\_len2 += (t2 \* t2);

278 }

279 return correlation / (sqrt(vector\_len1) \* sqrt(vector\_len2));

280 }

281

282 void CompareAllBacteria() {

283 Bacteria\*\* b = new Bacteria\*[number\_bacteria];

291 #pragma omp parallel for

292 for (int i = 0; i < number\_bacteria; i++) {

293 printf("load %d of %d\n", i + 1, number\_bacteria);

294 b[i] = new Bacteria(bacteria\_name[i]);

295 }

296

342 #pragma omp parallel for

343 for (int i = 0; i < number\_bacteria - 1; i++) {

347 for (int j = i + 1; j < number\_bacteria; j++) {

348 double correlation = CompareBacteria(b[i], b[j]);

349 printf("%2d %2d -> %.20lf\n", i, j, correlation);

350 }

351 }

352 }

353

354 int main(int argc, char \* argv[]) {

355 time\_t t1 = time(NULL);

364 Init();

365 ReadInputFile(argv[1]);

366 CompareAllBacteria();

367

368 time\_t t2 = time(NULL);

369 printf("time elapsed: %d seconds\n", t2 - t1);

370

371 system("pause");

372

373 return 0;

374 }