



IDEAL GAS SIMULATION

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Period 4

DESCRIPTION

- This program takes into account the temperature, pressure, volume, velocity, and number of molecules and uses the Ideal Gas Laws along with Maxwell-Boltzmann distributions to assign the appropriate values to the particles
- The animation itself consists of 12 discrete sequences that alternate in changing temperature, number of particles, volume, and pressure while keeping the dependent variables constant.
- As a result, we change one variable at a time and see the effect of the change on the pressure of the gas, which we can observe as collisions per second on the screen.

ALGORITHM SUMMARY

1. Color Algorithms
2. Velocity Algorithms
3. Ideal Gas (V & T) Algorithm
4. Ideal Gas (P & V) Algorithm
5. Random Velocity Algorithm
6. Bounce Back Algorithm
7. Volume Change Animation

COLOR ALGORITHMS

- A useful feature in showing relative temperature changes is to change the colors of the particles themselves. Our animation does this by taking temperature, linearizing the value to wavelength, and using a piecewise function to determine the color grade of the certain wavelength.
- This code is for the scaling of the wavelength to the r/g/b color values themselves. The values are multiplied by the max intensity and then raised to the power of the gamma factor.

```
270 //color of particles
271 double set_r(double temp){ //takes temperature as input
272     double G= .75; //gamma is set to .80
273     int MaxI = 255; //this is the maximum value
274     double l = 13*(temp + rand()%7 - 3.5)+ 380; //linearization
275     double red;
276     double green;
277     double blue;
278     double scale; //factor
279     if((l >= 380) && (l<440)){ //piecewise function
280         red = (440-l) / (440 - 380) ;
281         green = 0;
282         blue = 1;
283     }
284     else if((l >= 440) && (l<490)){
285         red = 0;
286         green = (l-440) / (490 - 440) ;
287         blue = 1;
288     }
289     else if((l >= 490) && (l<510)){
290         red = 0;
291         green = 255;
292         blue = (510-l) / (510 - 490);
293     }
294     else if((l >= 510) && (l<580)){
295         red = (l-510) / (580 - 510);
296         green = 1;
297         blue = 0;
298     }
299     else if((l >= 580) && (l<645)){
300         red = 1;
301         green = (645-l) / (645 - 580);
302         blue = 0;
303     }
304     else if((l >= 645) && (l<781)){
305         red = 1;
306         green = 0;
307         blue = 0;
308     }
309     else{
310         red = 0;
311         green = 0;
312         blue = 0;
313     }
314
315     if((l >= 380) && (l<420)){
316         scale = .3 + .7*(l - 380) / (420 - 380) ;
317     }
318     else if((l >= 420) && (l<701)){
319         scale = 1;
320     }
321     else if((l >= 701) && (l<781)){
322         scale = .3 + .7*(780 - l) / (780 - 700);
323     }
324     else{
325         scale = 0;
326     }
327
328     if (red != 0){
329         red = (MaxI * pow(red * scale, G)); //the value is multiplied by the max intensity then raised to the gamma
330     }
331     if (green != 0){
332         green = (MaxI * pow(green * scale, G));
333     }
334     if (blue != 0){
335         blue = (MaxI * pow(blue * scale, G));
336     }
337
338     return red; //returns red, the next two functions return green and blue
```

VELOCITY ALGORITHMS

- In real life, the velocities of gas particles follow a probability density function called the Maxwell-Boltzmann distribution, which is specified by the following formula:
- When you take the derivative of the distribution, you get a function for the x-value of velocity that has the highest probability for the particles to follow:

$$f(v) = 4\pi \left[\frac{m}{2\pi kT} \right]^{3/2} v^2 e^{-mv^2/2kT} \quad v_{rms} = \sqrt{\frac{3kT}{m}} = \sqrt{\frac{3RT}{M}} \quad \begin{array}{l} m = \text{molecular mass} \\ M = \text{molar mass} \end{array}$$

VELOCITY ALGORITHMS

- The root mean squared velocity is then used as the mean and the rest of the velocities are generated randomly around it, leading to a normal distribution if n (number of particles) is taken to infinity. Since we have a finite amount of particles, the approximation is somewhat crude but there exists a range of velocities nonetheless.

```
1105 particles[i].vx = rand()%(2*set_veloce(temp)) - set_veloce(temp);  
1106 particles[i].vy = rand()%(2*set_veloce(temp)) - set_veloce(temp);  
1107
```

IDEAL GAS ALGORITHMS

```
1250 particles[i].vx = rand()%(2*set_veloce((px*px)/vol*temp)) - set_veloce((px*px)/vol*temp); //use ideal gas law to set velocity
1251 particles[i].vy = rand()%(2*set_veloce((px*px)/vol*temp)) - set_veloce((px*px)/vol*temp);
1252
1253 particles[i].circle_color.r = set_r((px*px)/vol*temp); // set color
1254 particles[i].circle_color.g = set_g((px*px)/vol*temp);
1255 particles[i].circle_color.b = set_b((px*px)/vol*temp);
1256
1257 if(particles[i].vx == 0){
1258     particles[i].vx = set_veloce((px*px)/vol*temp);
1259 }
1260 if(particles[i].vy == 0){
1261     particles[i].vy = set_veloce((px*px)/vol*temp);
1262 }
1263 }
```

```
1101 for(frame_num = 900; frame_num<1099; frame_num+=2){
1102
1103     b_width = border_width + 200/198*(frame_num-900); //linearization of the border change
1104     vol = (px-b_width)*(pz-b_width); //volume calculation using cross sectional area
1105
1106     for(int i = 0; i < partnum; i++){
1107
1108         particles[i].circle_color.r = set_r(temp); //color assignment
1109         particles[i].circle_color.g = set_g(temp);
1110         particles[i].circle_color.b = set_b(temp);
1111
1112     }
1113
1114 }
```

- The velocities of the particles are set proportionally to both the volume and the pressure. If pressure doubles, the temperature doubles and the velocity increases proportionally.

BOUNCE BACK ALGORITHM

```
597
598     for(int i = 0 ; i<partnum; i++){//bounce back algorithms
599         if(particles[i].cx+particles[i].vx>px-border_width-small_radius){//if it hits a border, the velocity (either x or y )
600             //is changed and the ball collides and bounces back
601                 particles[i].vx*=-1;
602                 particles[i].cx=px-border_width-small_radius;
603             }
604         else if(particles[i].cx+particles[i].vx<border_width+small_radius){
605             particles[i].vx*=-1;
606             particles[i].cx=border_width+small_radius;
607         }
608         else{
609             particles[i].cx = particles[i].cx+particles[i].vx;
610         }
611
612         if(particles[i].cy+particles[i].vy>pz-border_width-small_radius){
613             particles[i].vy*=-1;
614             particles[i].cy=pz-border_width-small_radius;
615         }
616         else if(particles[i].cy+particles[i].vy<border_width+small_radius){
617             particles[i].vy*=-1;
618             particles[i].cy=border_width+small_radius;
619         }
620         else{
621             particles[i].cy = particles[i].cy+particles[i].vy;
622         }
623
624         particles[i].radius = small_radius;
625         fill_circle(buffer, particles[i]);
626     }
627 }
```

