The three-dimensional particle calculations that were shown in the previous sections relied on releasing thousands of particles to obtain a realistic looking concentration plume simulation. There is another approach in HYSPLIT that can be used, which is modeling the centroid position of the particles, by a single trajectory, and then also modeling how the standard distribution of the particle positions, within that centroid, or about that centroid, change with time. And computationally this is called a puff. So what we do is essentially follow a single trajectory, a single point, and then assume about that point a particle distribution.

So to get started with this calculation. Go ahead to the graphical user interface and since we've been doing a lot of different changes, go ahead and click the reset button to take it back to the test case. And then open the setup menu and we will retrieve the previously saved calculation, the particle calculation called part. We should also do this for the advanced menu. If you don't have this, we will review the configuration briefly.

Looking at the setup, the 25th at 17, Dayton, CAPTEX North American Regional Reanalysis data. It's a single particle release, fine grid spacing, half a kilometer, output every three hours, no deposition. So now to configure this with a different distribution rather than running as a 3-D particle model, go to the configuration, advanced configuration for concentration, and you can see in menu number three, we configure the release of either particles or puffs. And the default is to run the model as a 3-D

particle model both in the horizontal and vertical. We will start with something simple for the puff approach and we're going to assume a top hat particle, or top hat distribution in the horizontal but a particle distribution in the vertical. So what that means is we will only assume a distribution in a horizontal direction but in the vertical direction, the computational point will act as a particle. This can be more easily understood when we look at the output illustration. Go ahead and save and let's make sure we're just releasing one, for illustrative purposes, and will be menu number four. This one particle and let's now run the model with setup.

Now it appears for one particle, this is running much slower than the previous case. The difference between the 3-D particle calculation and the puff calculation is that as the particle or puff passes through the computational concentration grid, a particle is only sampled in the grid cell which it resides, whereas a puff, because it represents a distribution, contributes concentration to all the grid cells that are within the radius of the puff. Open up display, contours, and execute.

You can see here after three hours, this is the position of the single computational puff. You could go back and compare this with the 3-D particle, and of course the reason it took so much longer, is that you have this puff that now appears to have a diameter of maybe 20 km, 30 km, and there’s a concentration grid of half a kilometer, so there are hundreds, if not thousands of grid cells on here that the puff samples. And this is after 6, 9, and 12 hours.

Now here's a good example of why you may want to reduce the zoom, and let's also turn off the contour drawing option to none and redo this.

And let’s go to the end here and so even though were following this one particle, this one puff, it still contributes to many locations. And let’s change this. Oh, the other point I want to make here is that this is a top hat puff, which means that the concentration is the same at all locations within the puff circle, within that radius.

So let’s look at the other option under advanced, and menu number three. Let’s do a Gaussian horizontal, particle vertical, and run this again. Now this calculation is going to run even slower than the top hat for a couple of reasons. One is the Gaussian puff is larger, it's three standard deviations, is the radius, and also the Gaussian equation requires the complication of an exponential, which being for each of the grid cells within the puff needs to be computed, of course, at every time step.

And let's go and display, and it's not that clear here but if we go downstream, you can see essentially the Gaussian distribution, the highest values near the central peak and then decreasing out to three standard deviations. Now we can't see the vertical projection, but because this is a Gaussian only in the horizontal but a particle in the vertical, it has no vertical dimension. This is only a disk that is transported across the domain that bounces up and down in the vertical due to the turbulent velocities, intersecting different grid cells above the ground. The

model can also be configured as a three-dimensional puff model, but normally this is not used in HYSPLIT version 4. The three-dimensional puff approach is a legacy option from HYSPLIT version 3. The particle approach in the vertical is much preferable over or any puff approach because of the large shear in wind direction, wind speed, stability, that causes the vertical plume structure to be much more complex and therefore much more difficult to represent in a puff calculation. Whereas in the horizontal, a puff distribution is much easier to justify, because of the homogeneity in the wind field and turbulent field with respect to the distance scales that the plume would cover.

Let’s try one other experiment and let's go ahead and reduce the grid resolution to something not as fine, back to the 5 km resolution, save everything and then rerun the model.

Now, this ran considerably faster than the half a kilometer resolution simulation. Let's display the result, and you can see there is still the Gaussian shape but it has some noise at the end, you can see the grid resolution, the circle is not as smooth. If we go to the end, the inner contouring seems nice, it's only the outer edges that are noisy. But the complication of speed up was quite dramatic because of a really large reduction in the number of concentration grid cells. So having this simulation working, go ahead and save the configuration. We can use it later on, so set up, save as, and let's call this gauss_control.txt and the same for the advanced menu, this time it’s called gauss_setup.txt.

So before we conclude the section, let’s do one last simulation. Let’s increase the particle number, so instead of one particle or one puff, let's follow one hundred puffs. So open up the advanced concentration menu and set menu number four, the particle number limits, from one to 100, and rerun the model and then display.

So after three hours, it looks about the same, after six hours were starting to see some structure, and after 12 hours, you have an output that looks very realistic, and very much like the 3-D particle calculation. So in this particular simulation, 100 particles, or in this case 100 puffs, compare this calculation with the 100 particle calculation that we had done in an earlier section, and the particles of course, did not cover the spatial domain. We needed to run at least 10,000 particles to get this kind of smooth coverage. But a hundred puffs were sufficient and this provided us with a very realistic looking output and also computationally very efficient.

We will look into this … I'm a little bit more in the next section and this concludes the discussion of puffs.