**Modeling Neutral & Charged Fluids in VSim**

Hello, everybody, and welcome to the second day of TWSS 2021. We are so excited that you're here to join us we've had a very, very exciting event so far, we have now had people from 70 different countries login over the course of our event. So we're, you know, always happy to see people from all across the world. Today we have in the morning a series of short presentations. The first presentation that we have is Jarrod Leddy. He is a research scientist here speaking on modeling neutral and charged fluids in VSim, and Dr. Jared Leddy. He's been a research scientist here at Tech x for four years. And prior to that he received his PhD from the University of York specializing in of course, plasma physics. All right, Jarrod, I think that's an app. And one last thing I wanted to tell people actually, before I forget, we are going to be recording all of these talks, we hope to get them up to YouTube by next week, once we have them all edited, and processed. And then anyone who would like to receive an evaluation of our software can go online and request and evaluation through our website if you get excited with some of the stuff that you see throughout the event. So without that, I'm going to turn to turn it over to Jared.

Thanks, Colleen. I'm Jarrod Leddy. Like she said, I'm research scientist at Tech-X, I going to turn on my video and when I can, but for now, I'll just keep going. So I'm going to talk about modeling neutral and charged fluids in VSim, which is, well, those of you that are familiar with VSim you might know we've had neutral fluid capability in the software for years. But it's been limited in its capacity, it's been effectively static fields that you can use as reactants to generate, like ionization products or something like that. So for part of a research project I recently was working on. For the Department of Energy, we developed some new fluid models, one of which is where you have all the fluid via the Euler equations. And the other is a sort of MHD model. But it's hybrid. And it's something we can do nicely, because we already have the pick code, we can treat the ions kinetically. Still. So this is for problems where maybe you have you know, the ion dynamics are important to the physics. But the electron dynamics are less important, and so we can treat them as a fluid. Let's see. Okay, so for both of these, this now allows us to actually evolve the fluids, instead of having them just be some static field in the background of our simulation. And we've also included some more interesting boundary conditions than just slab boundary conditions. So you're able to model these fluids in your CAD geometries or interesting shapes, whatever it is that you want to do. And I'll show some examples of that. And another nice thing is that these fluids are CPU and GPU capable. So you can distribute them across whatever hardware you have, they haven't been released yet, they should be coming out with peace and 12. And I'll talk more about that as well. So just a little background, what I mean when I say the Euler equations. For those that aren't familiar, this is what we have. This is the system of equations we're evolving. So we have three fields, we have density, we have flux, we have energy for fluid, and we have all of them via these equations. And the nice thing about this is that they're all in kind of this conservative form. And so we can end up using a finite volume method nicely and easily for this neutral fluid. And so this is continuity equation, our momentum equation and then the energy equation. And we use this relationship and our closure here is kind of the standard standard adiabatic closure. The method we use to implement this is, like I said, finite volume. And so what we can do if this is our simulation grid and say we're looking at the center cell, we'll call it the other cell. We're using the standard muscle scheme to calculate the flux at the faces and use those flat face fluxes to actually evolve the field at the center point. And then these are numerical fluxes. And so we're using the lacs flux scheme where basically the numerical flux at the face is just the average of the physical flux, which is just the quantity times the velocity at the center of the neighboring cell. And so for example, the numerous flux at this face this high plus one halfs face is the physical flux at the center phase averaged with the flux of the face to the right. And then you have this extra term here, which helps with stability, which is phase basically the maximum flux. So, this is the scheme we used. And so I'm going to just show you a little bit in VSM itself. And so let me stop my share and then started again. So this is an example that will include in recent 12, with these capabilities, this is a Kelvin Helmholtz instability. And for those that are not familiar with this, effectively,

this is where we have some density of plot of neutral gas. And it peaks in the center, and decreases towards the edges. And we're using periodic boundary conditions on all sides here. And then, if we look at the flux, this is what kind of gives it this is what seeds the instability we have this shear flow. And so we have some, all the all the gases flowing to the right here. But you can see it's flowing faster in the middle, slower on the edges. And, in fact, it's got flowing in the opposite direction on the edges. And so we have this shear. In addition to that, we also need to see the instability with a little vertical perturbation. So this is the flux in the y direction. And you can see we're pushing this side down a little bit, and this side up a little bit. And this will give us just enough perturbation to see the instability. And we can see if I go back to the density, as we evolve in time, we get this sort of kink that forms and then we get the standard kind of Kelvin Helmholtz instability that that shows up. Just to give you an idea, this, I mean, I'm just running this on my local machine, it's 4000 steps to get this and it is pretty quick. So that's nice. You know, we can run that whole simulation to get the instability and 15 seconds or so. So we're pleased with the neutral fluid speed performance, and also its capability, it's getting the instability quite nicely. And it agrees with the theory. But this is all nice is a periodic box, you know, if you're doing some very theoretical stuff, maybe that's appropriate. But a lot of people are gonna have real geometries. And so we made sure that we implemented this, and this so that you can have cut cells, cells cut by whatever geometry shapes you want. And so I'll show a quick example of that as well. Let me share it. So this is a this is a shock simulation. And again, it's kind of a standard problem for benchmarking of neutral fluid models. But the nice thing about this is that the simulation domain is a square. But I flipped it so that we have actually a diamond simulation domain. And what we have is effectively a shock, where it's high density and pressure at the top load density and pressure at the bottom. And so we expect a wave to propagate down and then behave accordingly as it reflects off of the edges of our box. And so we can see that is in fact, what happens, we get this nice symmetry that doesn't break throughout the simulation of these waves bouncing around our rocks. And so this we can, we've benchmarked against, you know the other other codes that do the same type of problem and find that we agree quite well in time. And importantly, one of the most important things is that we don't lose the cemetery and the simulation that means we're treating the boundaries correctly. So, that is where we are with the neutral fluid model and as I mentioned before, we expect that to come out in the next major release. So for those of you interested in modeling neutral fluids, alongside the other capabilities of the SEM you will be To do that, so that's the neutral fluid. I want to talk a little bit about the hybrid fluid model. And this is a bit more challenging than the neutral fluid models, you know, neutral, neutral fluid models have been around for a long time. These hybrid fluid models, in theory have been around for a long time. But in practice, you know, people are still releasing research papers, modifying algorithms and things like that. And so

like I said before, sometimes the electron timescales and behavior are not important to the physics that you have in your problem, but the ion kinetics are, and we particularly maybe care about the ion kinetics because the non maxwellian are there Do they have, you know, large tails, things like that. And so in these cases, we want to have kinetic or pick ions, we'd like to be able to skip over those fluid timescales, like the electron timescales. So by treating the electrons as a fluid, were able to increase the timestamp decrease the spatial resolution requirements, because Dubai is less important. But we are making an assumption. And so we have to be careful about which problems we can apply this to. Again, some equations, but this is just to give you an idea we're treating ions is kinetic. So this is just literally the kinetic equation for the ions. We're using electric and magnetic fields. The important stuff, the stuff that makes this different, I suppose is the electron fluid. And so we only have one equation for electrons, which is, we're solving for the pressure the electron pressure here. And this is a fairly standard pressure equation. You know, we have viscous heating and heat flux and everything else is is pretty normal. But importantly, this is an electrostatic type model. And so we calculate the electric field from ohms law. And so we can use the information we know about the ion. So there's like the eye we're getting from the kinetic ions themselves, along with the J, the grad P, and then we do have a magnetic field, but we're calculating it from the electric field we get from ohms law. So this is the system we're solving. And this is from the stanier paper in 2018, internal computational physics. So it's not something the model itself isn't something we developed, we just implemented it. And one thing you'll notice, so we if we have kinetic ions, but then we use something like the ion velocity in a, an equation to calculate the electric field on a grid, that means we're having to take moments of this kinetic distribution. And so we are able to take our ion kinetic information, which is just a bunch of particles at random location that you know, at non grid point locations, and we take averages those and deposit them onto the grid, so that we can use these field quantities like VI and J, and the density as well, are all taken from these these moments of the Connecticut equation. So we implemented this, and then we wanted to benchmark it to make sure we're getting correct answers, because that is important. And so we expect that this hybrid model should in some cases, anyway, some physics problems give as good an answer as pick with increased speed. And in some cases, we also expect that a full fluid approximation would be incorrect. And so we're kind of sitting in that middle ground where we're trading performance for accuracy, but not accuracy, because we're putting it to the right problems where we don't care about those electron dynamics as much. And so, some of those problems are this ion acoustic Landau damping. We because the Landau damping is done on the ion timescales and because of kinetic ion effects, this is a good choice for applying this algorithm. Likewise, the gem challenge problem problem, which is a reconnection problem is also appropriate. So I'm going to go through these two examples and just show you some of our results. So you can see that we're, we're, our implementation is accurate. So just a review of what Landau damping is you have we have our setup. Anyway, for this problem. We have a thermal plasma, and it has a density perturbation at the ion acoustic wavelength. And this results in an electrostatic ion acoustic wave. So we add we add this perturbation at the right wavelength and we expect it to oscillate up Because of kinetic ion effects, this oscillation will be damped. And the oscillation will shrink as the ions effectively take energy from the wave and from the electrons. And this damping rate and oscillation frequency are known from theory for this type of problem, which is why it's a good benchmarking problem.

So, I guess, so I can show you these plots, but also pull up VSM. This is the electric field in the center of our problem. Actually, what let me pull up the sim first because I think it would be useful to see the initial setup. So let's go here. So we're setting up a perturbation. That is roughly the wavelength of our box, which also we've designed to be the ion acoustic wavelength. And so what would we expect is that this, also, this perturbation oscillates in time. And we can see that is what happens. And the wavelength stays constant, it's just we get this oscillation. But you'll notice the oscillation is indeed shrinking. And that's what we expect. And what we want because we what we want to do is measure the rates at which that is damping. And so we added a history to look at the electric field at the center point. And here's our oscillation, it's nice and an even it's at a particular frequency. And you can see it is damping. And so I can take the log of that. And while that is not great, let's put this man at minus six, you can see we have this nice exponential typing rate, linear in log space, which is what we expect. And that's the plot I was showing on my slides as well. So let me pull those back up. And show you in more detail some of the results. So we have, again, this that same plot the damping tapping on a particular frequency, we can FFT this to get the frequency. And then we can fit that history that I showed you. So there's the history, you can see that same oscillation is damped. And we fit that. And we know the theoretical damping rate. And we can see our damping rate, and we're within 15%. And so that's not bad. And we can also do things to improve this. So, Landau damping simulations are notoriously noisy. And so one thing you can do to increase the fidelity of such a simulation is increased particles per cell increased resolution, that sort of thing. And so there are ways we can we can refine this simulation, but I think it shows one that we're capturing the physics that we should be. And to that we're doing it to a fair degree of accuracy. And this is particularly for some t over t is five, which tells us that we're saving quite a bit of computational speed by not having to resolve the electron timescales, the electron timescales, if the energies or temperatures were equal, would still be we'd be saving roughly 40 times with a speed in you know, being able to just resolve the ion cyclotron time instead of the electron cyclotron time. At t over t is five, we're getting roughly five times that and so we're getting a significant savings by going to this hybrid method. So that's the Lando damping. I want to talk a little bit about this gym challenge as well. This is like I said, a reconnection problem. And so the setup here is that we have a current sheet, you can see the we have an electron pressure and density that peaks in the center. And this all has some velocity into the page. And what that means is that above this sheet, we have some positive magnetic field that's being generated by this current density. And below the sheet we have a constant negative electric field. So pointing to the left below right above. And this is actually a stable configuration. If we have an ideal plasma, but plasmas are not ideal. They have resistivity and other kinetic effects and we expect that this will become unstable in those cases, and it will be kind of unstable and what we should get is effectively some b y Some vertical magnetic field that starts to form and will get islands that develop in this in this type of situation. So magnetic islands. And so we

do indeed see that happen. And so this is b y, this is the vertical magnetic field. And we would expect with this starts off exactly zero. But over time, we get this b y that starts to develop due to these kinetic effects and resistive effects. And that's what's giving us our islands, then if we have that Bx, and we have now a, b, y, we'll get some sort of shape of magnetic field that is, well, Magnetic Island in nature. So we'll get that reconnection that starts and we can measure this integrated flux. So this is the flux in the y direction, integrated across the x domain. And then we can see that at time zero, we have no magnetic flux in the y direction. But as the reconnection starts to occur, we get this significant increase. And we can look at other papers that do this kinetically. And we could even model it kinetically in VSM. And we see this same rise and the same time, I will say that we ran this with 20 particles per cell. And to give you some context for the Landau damping, we ran 50,000 particles per cell. Because lambda damping is quite noisy. It turns out this is also a little noisy. And so after the reconnection starts to happen, there becomes a there we reach a point where the noise is too much. And so the magnetic flux starts to fall, we're really we would expect it to remain roughly constant. And so this is again, something that we could expect to increase particles per cell and see, see this fidelity maintained further and further. There are also things you can do with having very quiet initial condition starts for your particle positions and things like that, because we're doing all this averaging, this moment taking to get electron density, energy ion density and ion velocity. There's some intrinsic noise in these types of simulations. And one thing we do to remove that is we smooth the fields. And this is again something that they do in the paper and I can show you real quick, the CIM challenge. So here is the sim. You can see we have all these fields in the hybrid model, we have magnetic field, we have current density electric field, we have the resistance resistive lis electric field, current density ion current density, we also have this smooth versus the non smood. And you can see, perhaps, the difference it makes to smooth versus not smoothing. And this is kind of necessary to you know, get the noise to average over the noise a bit. And is, if done correctly, should not affect the accuracy of the results. And so again, you can see all this in that standard paper if you're interested. They also do the smoothing. So think let me share my slides again, I am nearing the end here. Yeah. So in summary, we have vsam 12, that's going to be coming out with the ability to evolve fluids. And this is something new to these. And these fluids can be both neutral and charged. I will say the charge is it's a specific model, right? It's this hybrid model. It's not just generic charge fluids. But it has a specific application that we find useful if you want to do full fluids. For charge plasma fluids, then we do have a product for that as well use m so the fluids can be evolved in periodic slab geometry with slab boundaries or even more complicated geometries. Just a note, in case you noticed, I didn't show you much of the actual setup, but the everything I showed him today wasn't text setup, but it will be in the GUI for VSAN 12. So never fear. And that's all so if you have any questions, I'll be happy to answer them. And thanks for listening.

Very good. Jared. It's always neat to see what's coming down the pike great. If anyone has questions, there is a q&a box at the bottom of the screen and you can type them in there and we will read them And be able to answer them. Well, Jared, well me. As I said before, this talk will be recorded and put up on YouTube. So hopefully by sometime next week so that you can refer back to it if there was anything else that you wanted to see a second time. And if you are interested at all in evaluating vsam vcm 11. If you haven't tried the newest version, if you go to the tech x website, at t x Corp, comm TX Corp dot c om, you can request a 30 day evaluation of the latest version of any of our software. So and it looks like we have a couple of questions to start out with dirt. So the first question is, can the electron fluid be given a drift velocity.

So we initialize the electron fluid with just the pressure because that's the only field we have for the electrons. The electrons we assume to be calculated the electron velocity we assumed to be j minus vi or n vi. And so you could set up an initial current density fields and initial give the ions an initial velocity, and the difference between those will give the electrons some effective initial velocity as well. So if that's, if that's what you're looking for, then yes, we can do that. Where is that? Oh, if so where's that term? Yeah, so I can go back to those equations. But, um, I didn't show a couple of things like j is in vi plus NB. And so that it allows you to do that calculation that I just mentioned. But so so like this V here and the P equation that is calculated from j minus NBI. So yes, I think you can give it you can give the electrons some initial drift velocity relative to the ions. But it's not as simple as just you know, specifying the and then Ming che, did you ever compare fluid or hybrid model with pure pick? So we did do? So for the Landau? We did? So okay, so there's a couple things. Yes, we did for some established pic results. And they agreed. So if I show you, for example, what the Landau damping they agree very well, the gym model, they agree up to a point, and then we lose some fidelity, whereas the pic would have stayed up a pie after this. And we did also try and do Landau damping in VSM. So our own pic results to compare with the Landau damping. It's just very expensive to doing Landau damping and kinetically, especially if an ion acoustic wave is very expensive. And so and also quite noisy, you need to use many 10s of 1000s particles per sell. And, you know, we ran it and we saw agreements, up to maybe the third peak here. And then the pictures flattened out and got noisy, whereas the hybrid stays quite nice for for much longer. So yes, we did do the comparison. And we see we see good agreement, especially with the lambda damping, and up to a point with the gym. The other question beats on 12 be released. I can't give a firm date on that. But it's our next version. And we have some good features for it that we expect to be out. You know, either the interview this year or early into next year is is the plan. So we'll see how that goes. So Udo asked, Can these initial conditions for electrons be exported from a fully kinetic pre run? So yes, for sure they could be. If the question is, if it's automated, and something that you could just like have vcm do as of now, no, but maybe that's something we could look into actually implementing because that could be interesting to be able to do that kinetic initial run and then switch to hybrid fairly seamlessly. But right now, no, you'd have to, you'd have to do like, some analyzers to get that data. And then yeah, you could import them as like pi funks. And that sort of thing into into the fields that you want.

So there's another question that talks about how will this worked with particles I don't know if you've

seen so the hybrid model uses particles it uses kinetic particles. I guess Now, I can show you real quick the simulation for Jim. So you'll notice I have all these fields which are rough, these are kind of fluid fields. But I do have particle data up here as well. And so we can look at the ions specifically and see how they evolve. So this is the, so it starts off nice and clean as you'd expect from my kinetic simulation, and then the particles start to move around, and we see the pressure, the density, diffuse, and also obtain some sort of perturbations. And so the hybrid model does use the the does use kinetics, if you're talking about the neutral fluid model, the way you would interact with kinetics would be through the reactions framework. And so you could have if you had like a neutral fluid background, and so you had some kinetic species that were also you expect the kinetics of those species to be important, then you could have them in the same domain. And then you would just need to specify reactions between them, whether it's elastic, or ionization, or whatever it is, that would allow the fluids to interact with the kinetic species.

That answers the next question, which was how will the neutral fluids work with particles? Good. And it looks like another question. So how many particles per cell Do you need to run with for the hybrid model?

It depends on the problem. I said, for the Landau damping one we ran with 50,000 particles per cell. And so is a lot but that's because Landau damping is quite a noisy problem, the gym problem we ran with 20 particles per cell. And maybe we should have run with more. But I don't think we need to go as high as the the lambda damping problem, right. So there's not necessarily a strict and fast rule for how many you need. But because we're taking these ion kinetics, ions, and taking the moments to get the density and things like that there is the more particles you have, the less noisy that'll be. So you can see, for example, here is the kinetics, these are this is the weights that I'm plotting and so higher weights are localized here, we would expect to see this same type of shape, if I go and look at the ion charge density, right, so I can click that. And we'll see. Let me turn off those, you can see that same distribution is showing up. But it is somewhat noisy. And that is because we are using 20 parts per cell instead of maybe 50 or 100. And so it's always a bit of a not a game, but you have to just play around with it and see, you know, how smooth Can you get it? Without? You know, we're balancing the performance and the computational cost? And I think that's the same with I mean, that's kind of the game you play with all simulations, you know, what resolution Do you need in order to get accurate results? But without detrimentally affecting your computational performance? So it's the same type of thing here. Daniel Han says, Can the initial line distribution be loaded from file? And this is specifically for the hybrid model, I assume? And so, yes, it definitely can be. I guess it depends on what type of file we're talking about. You could load it from a vsam file, no problem. If you had some theoretical functional form for your distribution, you could also do that. I think if you're getting your ion distribution from I don't know another piece of software, you'd have to figure out a way to either like fit it and use that fit function to load the distribution into V center or something else. But yeah, that's, I think that is the are all the different ways you could you could do that. Ming che will the fluid models work correctly for particle collisions with a moving fluid? Yes, that that is the hope I mean, they should do because all the reactions are local, right? We the way we do the reactions is by looking at the, the fluid in a cell or the reactants basically in a single cell. And so in this case, would be a fluid reacting with a kinetic species, perhaps. And so, the way we then do that is to sample the fluid distribution to get some sort of pseudo particle that has, you know, the right velocity Based on the fluid velocity distribution, the right weight based on the density, and we interact that with the particle, and then we feed that back into the fluid and the particle. And so if the fluid had some initial velocity, like some flow rates to a particular direction, and we would expect a momentum to be imparted to the kinetic species as well, yes.

So we've had some great questions today. Very cool. So if anyone we've got Jared for a few more minutes, if you have any last questions you want to ask, before we take a break until our next presentation. Thank you so much. As always, like I said, it's always fun to see, you know, the development pipeline and and what else we're going to be offering as well. So okay, I think we'll go ahead and stop there. Thank you so very much, Derek. That was, thank you for taking the time to do this. Our next presentation will come up in about an hour. So we will have at that time, Luke Adams is going to be presenting a presentation on grid instability, growth rates of electrostatic particle and cells, elation algorithms. Oh, we did get one more question which asked about will that feature be available in recent PD?

I so the Euler fluid I think we're going to put in be some base. And the hybrid model will be NPD. That is my understanding. But the we haven't officially decided on that. So. But that's, that's I'm pretty sure the way we're going to go with it. Yeah.

Okay. Great. All right. Well, thank you, jer. Thanks everyone else who has joined us so far. We will see you in about an hour.