**IBVRE Study Trip to Washington and Lee University, Lexington, Virginia**

Day 3 - 31 January 2006 - Demonstration of UI Mockups to Ashley Brown and James Eason

Present: Ashley Brown (AB), James Eason (JE), Clint Sieunarine (CS), Matthew Mascord (MM)

Before the UI mock-ups were demonstrated to Ashley Brown, a couple of changes were requested by James Eason:

- Jamey felt that there wasn't a need for a set of Run buttons on the were redundant.

- That the three tables on the View Experiment page could be replaced with a single table allowing the strength and time to be specified as a single value or as a range. This introduced the need for a No. of Times and No. of Strengths column

The following is an edited transcript of the conversation resulting from MM demonstrating the mock-ups to AB.

MM: So we came up with view study, set up study, create a series of experiments. We're going to get rid of the 'run' column.

JE: So a study would be comparing waveforms or comparing epsilon, the study involves the whole thing, each experiment is essentially one of your [i.e. Ashley's] letters. A would be an experiment.
MM: So in the edit experiment you'd be able to set a range of times, the minimum time you can specify for any given simulation, range of strengths similarly, maximum shocks, so when you add up all the shocks it will never exceed that number. All will be fixed for each simulation you do: tilt, dt, epsilon, waveform, duration etc.

MM: To set up the experiment you'd set up a series of batches, a series of shocks, a column or a row, or a grid, you could specify a single strength and time in which case it
will be a single shock or you could specify a range of strengths and times, in which case it will create a grid based on how many strengths and times you want.

AB: So when it says number of strengths?

MM: How you want to divide it up.

JE: For your purposes, would it make sense intervals, or the difference in strength?

AB: For me it makes more sense to have the difference, every 0.1. It makes more sense to me, rather than having to divide. I have problems with end points.

JE: As soon as you enter one it will calculate the other.

AB: The results, what would that take me to?

MM: It would allow you to download the results. What form would you want the results in?

AB: It would depend on what we are doing. I feel most would be ED50, so I guess ideally I would want to directly import into JMP.

MM: So you'd want post-processed data?

JE: Would it be possible on the results, to give either give a list of files or give the option of saying you want everything, or just results.

MM: So a series of different post-processing steps?

AB: I feel sometimes you want to look at the simulations, watch it in 3D, but for the one I'm doing now I just want to know the ED50.

MM: So you'd be able to specify that somehow.

AB: So as an example how would I use the batch part, or would it be necessary to break this down?

MM: Are you doing shocks there or multiple?

AB: Multiple.

MM: So you'd set up a batch, fixed strength or fixed time.

AB: So I'd need one batch per experiment?

MM: The only difference between batches is granularity.
MM: You'd only need multiple batches if you need different granularities, is that something you do a lot?

JE: But that's something you did. You looked at fine detail at particular regions for one version of the study.

JE: You might want a finer spacing in a narrower version.

AB: So whenever you, if you click on edit, under edit experiment.

MM: So you're setting up things you can't change for each batch.

AB: So range of times - is that range of start times?

MM: Yes, the minimum. You can't create a batch with time lower than 2.6. All your ranges have to be between 2.6 and 3 ms.

AB: So that's the start time, if you start the simulation at 3 will it go past 3, or will the entire simulation ... ?

JE: For example I might set this as a hard-coded limit between 2.6 and 3.0 because those are the only restart files I have, so you can't accidently go in and set it for 3.1 because I know I don't have a restart file there. [MM: Needs clarification.]

AB: And the duration, what is that?

JE: I was thinking that was the duration of the monophasic shock.

AB: So what's the duration of the simulation?

JE: That's not currently a variable.

MM: The idea we would capture things that are applicable for 80% of experiments. Will these cater for 95% of experiments?

JE: The simulations you're doing now, you'd need a dt1 and dt2.

AB: And then you can't change the waveform?

MM: You can but you'd have to create another experiment.

AB: How do you do that?

MM: There'd be an add button, but for a single grid it would be only monophasic or biphasic.

AB: And it would automatically ____?
MM: Yes.

JE: Is it saving it in a particular format, is it like in XML?

MM: It would go to a database and you could extract it.

JE: So you could have a script that.

AB: What about the nodes? How many nodes are we going to use?

JE: This is the thing we're talking about with Rance, how we're going to do the job submission, which nodes.

MM: Is this something you'd need to control?

JE: For instance, you're only going to be running from 1 to 16 and Rance was saying that we could start a virtual machine, and leave it running, so that whenever you submit these jobs, it runs on your virtual machine, which is limited to whatever, 1 to 16, so you wouldn't have to go in each time and restart do the lamboot stuff, you would start once, leave it running, this would connect to the machine, and submit to virtual machine. So if you were already running something, and you submitted over and over, it would resend and you'd have 10 jobs all running on your small machine.

AB: Is there a way to tell if the jobs have done, or would I have to SSH in there?

MM: So you'd need a status?

AB: Or a big green checkmark.

MM: So we've got a run button here so you can run them individually or all at once.
Fig 4 - Demonstrating the run button on the view experiment page.

MM: Is it a valid thing to be able to run them individually?

AB: Yes because if it's going to slow down running them all at once, I'd want to be able to run them individually.

AB: So you could have them all ready, but ... .

MM: We could have a separate box underneath saying which jobs are running, or we could include it as a column.

AB: I think a column would be good, and you can see submitted, or run.

MM: So you'd never have to go onto the shell, that's the idea.

JE: And also think about what would help think how you would get Matt [Kolansky] to do what you're doing. Without having to teach him all these little details, learn UNIX, this and that, how could we take someone who is even less computer literate than a biology major, english major and make them useful in the first week.

AB: I think definitely the increment thing, instead of the number, either up to this, or, start here with increments of this. Either up to this or ___

MM: If we got something working by the end of the week, would you be able to see if it makes sense?

AB: I think it's pretty self-explanatory. If you don't have to figure out the nodes, JE: That's something we've still got to work out, come to an agreement with Rance, figure out how to do what he suggested.
MM: So what form would you want to download your results? A spreadsheet, CSV?

AB: Do you think a spreadsheet that you can import right into JMP?

JE: I'm sure we can figure out what that format is, it's probably tab delimited or something.

MM: If it's CSV it'll automatically load it up.

AB: Columns with time, strength, outcome.

JE: If we're clever enough in the script we could generate that in the script, I'll try to figure out what the format for that thing is.

JE: Would you find this limiting in any way? Would you use something like this get annoyed with it because, or is it a matter of trying it first?

AB: I'd have to try it - it sounds good, for what I've been doing. The thing back on experiment, total number of shocks, so if I had different batches that exceeded, what would happen?

JE: It would charge your university card account!

JE: That was just my thought to make sure you don't submit 4000 jobs.

AB: What if you want to kill a simulation? I never remember how to kill something.

MM: So button to see kill?

AB: Maybe underneath the status box.

AB: It should ask 'Are you sure?'

JE: So each batch will have its own CSV file. I was wondering if we could get JMP output that ED50 without copying and pasting it or even go in there. I'm pretty sure there is a command line interface to that. It's just a graph interface to it.

MM: Well that would be ideal, cuts down the number of steps.

JE: Exactly.

AB: So if you want to run one shock on Euterpe, can you do that?

MM: Well you could just run one shock on there.

JE: This could be the resource thing.
MM: Well that's the whole idea of globus, it's transparent.

JE: Another iteration add in the flexibility to do that.

AB: Actually that wasn't my question. Are we going to store the shock files?

AB: Will we know where that is? Will we get to specify 'Put it here'.

MM: I was thinking we could download in different formats.

JE: Is it going to put it somewhere?

JE: The other thing, so this thing is going to automatically store a bunch of files to the cluster. So we know something doesn't work, and we're done with it. Would there be a way to erase things?

AB: I think under the experiment level, have something.

MM: Is it enough to download from web portal or OK to log in.

AB: I'd want to log in.

JE: So perhaps it should be a variable in the experiment level, where you say save the data or not save the data if not save data, it would throw away post-processed thing.

MM: The idea is to minimise, eliminate need to go into the command line.

AB: If I did need to go in I'd need to know where it was stored.

JE: We could send all this to a place not backed up, I don't know whether it would make sense to put it on a temporary disk that would be erased.

MM: Could flag stuff as deleted, keep the metadata, have a cleanup task.

AB: Is each person is going to have their own login to this web portal? So I go in and see the experiments I'm working on? But Matt [Kolansky] will have his own. I can see us getting a lot of experiments.

MM: That's the other issue, versioning of experiments.

AB: Would it be worth separating it by month? Have an initial menu where you can look at this month etc. Or it will come up for this month by default.

MM: Remember you're ordering it by study so you're going to start off with a list of studies and presumably not going to build up hundreds of experiments for one study, so there's a certain organisation.
JE: If it showed most recent first?

AB: OK.

MM: Does it need a timestamp to say when created the experiment.

JE: Not a bad idea.

MM: And what about when you ran the experiment?

JE: I'm not sure I'd ever look at it, but there could be a time when it'd be interesting.

MM: I think the important thing is so you don't lose any history. You don't lose the fact that you ran the experiment on this date.

JE: I like that, the idea of logging everything.

MM: It shouldn't be a huge storage issue, you're only storing metadata.

JE: Exactly, and this is all in the database, and there's plenty of ways you could look at it.

AB: You could analyse it to see how many simulations did I run this month, or was I slacking off!