

Hi, people,

This is a letter about computing, software we use, our cluster, and the interaction with ChemIT people. I write it because there are new people in the group. And everyone comes here from a different computer environment, and places that are more or less (likely more) rich in computational equipment and staff to help with programs. Or they may come from larger groups, where there are people in the group whose job it is specifically to help with software and programs.

Basic principles, in plain English:

1. We are a group. That means we share everything computational, and help each other.
2. You have to make a *bona fide* effort to install any new software.
3. ChemIT people will help, of course. But they are not there to do it for you.

Now let me flesh out the consequences:

A. You are responsible for installing, configuring, and knowing how to effectively use any research application you use. You can request assistance from Lulu, but only after you have made a good-faith effort to learn and try to fix any problem. I know this takes time, but I assure you that the skill gained will stand you well in the future. Lulu can contribute to expanding your knowledge of something you are responsible for understanding, even as she assists you in getting things working, with your active involvement. The effort on your part and active involvement are essential.

There are also former group members with special aptitude for getting programs running. We can't ask it of them, but often they are willing to help. Ask around in the group who they might be.

B. Putting programs or software in your home directory that might be used by someone else in group is not sharing. Application software you install on the cluster, if it has even a remote possibility of being used by someone else in group, should not go in your home directory. It might initially, but when it is operational, it should be installed in /home/hoffmann/bin. If it is new, send an email to the group telling people about it.

Let me put it another way: As people leave the group, and new people arrive into the group, their home directories won't have software others depend on. For these reasons, if Lulu is asked to assist in application installation, configuration, or use, the assumption is that the application is for group use, and will appear in /home/hoffmann/bin. That also goes for any useful program you create or compile yourself.

C. There may be a gray area for programs that you have which were obtained without a proper license. Come and discuss them with me.

D. ChemIT has drafted a page listing the research applications (and related software), identifying explicitly the software they and we are responsible for installing (including compiling) and maintaining: <https://confluence.cornell.edu/x/lwEoDw>. One consideration at work is that if a program is used by several research groups, ChemIT likely will take over responsibility for installing it, but that if it is used by just our group, the primary responsibility is ours.

Even for software ChemIT is responsible for installing, you as a researcher still have the responsibility to know how to effectively use the software, to confirm it works correctly (and helping characterize the problem when it doesn't), and for thoughtfully responding to requests related to ChemIT's debugging efforts of that software to meet your needs.

E. Please continue to send the initial request for help at <ChemIT@cornell.edu> or by using their web form <<http://it.chem.cornell.edu/request/>>, particularly if you are not using Cornell's email.