From: David Cook <david.m.cook@lawrence.edu> Date: April 4, 2007 12:56:50 PM EDT Subject: A start on the PICUP Workshop

The PICUP WORKshop at Argonne is now only a month away, and I would like to begin a conversation about the contribution of Group 3, the group in which you have agreed to participate and that I have agreed to convene. As you probably recall from the invitation, Group 3 is to focus on designing one or more prototype computer-based modules that could be used in an intermediate or advanced course in electromagnetism, perhaps as homework exercises, perhaps as in-class presentations, perhaps in some other ways. If you have not already done so, I suggest that you look at the PICUP web page

http://CompPhysEd.shodor.org

and, in particular, that you look at the paragraphs following the tentative schedule that comes up if you open the link to the provisional agenda/schedule. Those paragraphs describe the expectations we are placing on each Work Group more fully than I have here.

With this email, I would like to start a discussion among the three of us that will perhaps lead to the identification of a number of possible topics for the modules we develop and, maybe even more importantly, to the identification of a number of broader questions whose answers may influence the detailed structure of the modules. For example, I think in broad terms that we ought to think some about how to balance using a computer to learn about some physical system and using some physical system to learn about computers. On the one hand, an approach that focuses on the physics without giving explicit---and in some cases fairly detailed---attention to the tool is, I think, in the end not completely satisfactory, since it risks developing an incomplete appreciation of the capabilities of the tool. On the other hand, an approach that focuses on the tool without leaning heavily on the physics for motivation is also not satisfactory, because it fails to provide the contexts in which the tool has application. In designing effective homework exercises and classroom components, I think we need to worry as much about how students will learn about the tools as we do about the physics that they will learn in the process.

By way of suggestions for possible topics of exercises, I am attaching a memo that I prepared a month or so ago and distributed to the members of the steering committee. There is nothing particularly profound in these exercises, and many can be done (tediously) without a computer, but I think they provide a basis for learning some physics while at the same time learning about the tool. Assignment of any of these exercises would require some prior discussion of the appropriate capabilities of the computational tool to be used.

I hasten to add that these exercises are merely suggestions. With this email, I solicit your beginning thoughts about possible topics for modules and also about broader questions that we should include for consideration in the meetings of our Work Group, once we all arrive at Argonne. I would like to have something of an agenda for our group laid out before the WORKshop begins so we don't spend too much of our valuable time together figuring out how to start. I would like to try to do that before we gather at ANL.

Further, if you already have exercises and/or modules that you would be willing to have linked to or mounted on the PICUP web site, please let me know.

As you probably both know, using computational resources in upper-level physics instruction has been a particular hobby horse of mine for decades. I am excited that steps are now being taken to try to speed the process of integrating serious computing into the undergraduate curriculum across the country. I am hopeful that this WORKshop and the activities that follow from it will constitute positive and effective steps toward the attainment of that broad goal. I

thank you for your interest and for your willingness to participate---and I look forward to hearing your thoughts on the more immediate task that confronts our Work Group.

Sincerely, David

PS: Just in case you don't already know each other, Jan is Jan Tobochnik at Kalamazoo College and Editor of the American Journal of Physics; Kelly is Kelly Roos at Bradley University; Norman is Norman Chonacky, editor of Computers in Science and Engineering and, with David Winch, now retired from Kalamazoo College, is the prime mover behind the creation of PICUP.

From: Michael Gray <gray@american.edu> Date: April 4, 2007 3:45:13 PM EDT Subject: Re: Invitation to a workshop on envisioning computing in undergraduate physics

I'll be delighted to attend ! This workshop is exactly what is needed to rethink how we can get a stronger computational basis in undergraduate physics. Group 3 is a good group for me since I've recently taught upper level electromagnetism to our physics majors here at AU and since I have a strong interest in computational approaches to electromagnetic propagation and scattering.

From: Jan Tobochnik <jant@kzoo.edu> Date: April 6, 2007 8:29:34 AM EDT Subject: Re: A start on the PICUP Workshop

Dear David,

Thanks for reminding me of what group I am in. E&M I think might be one of the toughest subjects to make a real impact at the undergraduate level because the principle goal of the course seems to me to teach what a field theory is all about and to help students become more proficient in solving pdes and doing vector calculus. Of course all of these can be done on the computer, but then we have to be careful to make sure that the students lose out because too much is done for them. However, there is also one opportunity and that is visualization, which seems to me to be more important in E&M than just about any other topic in physics. My experience in stat mech is that talking about algorithms contains a great deal of physics. I gained a great deal of understanding of what probability and the Boltzman factor was all about by learning the Metropolis algorithm. I think the same may be possible for thinking about visualization algorithms in E&M. Up until relatively recently visualization was to computationally intensive, but I think computers accessible to students are now fast enough that it should be a key part of what we do.

From: "Roos, Kelly" <rooster@bumail.bradley.edu> Date: April 10, 2007 2:09:50 AM EDT

I've decided to disclose my zeroth order thoughts on the matter in order to contribute something without letting too much more time pass before responding. I plan to consider the tasks facing our work group further over the days to come, but here are some immediate ideas that I have regarding integrating computations into the traditional format of an E&M course. David, I have decided to not read your assignments memo until after I have written this so that I could come up with something close to original. I did however read your's and Jan's email messages, and concur wholeheartedly with the concepts of giving equal emphasis to the physics and the tools used in the computational solution to a particular problem, and that E&M provides an excellent opportunity for students to explore visualization of a field, and to learn

computational visualization tools.

The first assignment I would have the students do would be to model a classical H-atom, even though it could technically fall under the classical mechanics category since the physics is the same as the 2-body planetary motion problem. Depending on the students' level of computational experience they may or may not have done this particular problem before. If they haven't seen it before, it would serve to warm them up to some of the concepts in computational physics; in particular, the simple application of the first order Runge-Kutta method and learning to develop some programming savvy, or the nuances of a particular commercial software package. By the way, I have extensive experience integrating computational assignments into classical mechanics and statistical mechanics, and my style has been to require the students to program everything with a language such as FORTRAN or C. This approach usually requires a significant effort on my part in providing extra training to get the students to the point where they are sufficiently competent to carry out the programming on their own, and on the students' part in dedicating themselves to learning the language on top of the other analytical requirements for the course. This brings me to a specific question I'd like to pose to the group: what computational vehicle should we advocate--direct programming, or a commercial software package, or both? I suppose that visualization of a field would best be accomplished with an available software package.

But even if the students have done the Kepler problem computationally before, I would still have them do the H-atom as a good review. And then, perhaps, have them "graduate" up to the more challenging mechanics problem of modeling a He-atom. Though it would be essentially a 4-body problem in mechanics, there is the extra interesting phenomenon of 2 sets of different charges interacting (there is only one kind of mass in the gravitational multibody problem).

After the H and He-atom warm-ups, until the point in the semester is reached where the students learn about solving boundary value problems, I think the best integration of computational physics into the E&M course would be through the visualization concept that Jan mentioned. There, of course, are many problems involving the field produced by different charge distributions. These are perfect candidates for using the computer for visualization.

The following is a short list of computational assignments I would suggest for boundary value homework problems or classroom demonstrations:

- Solve Laplace's equation numerically (introduce the Jacobi method, or some similar relaxation approach for solving a partial differential equation) for a particular boundary geometry, and then create a 3D visualization of the resulting equipotential lines and field.

- Solve Poisson's equation for a particular charge distribution and set of boundaries, and then do the associated visualization.

- Calculate the magnetic field of a solenoid (introduction to numerical integration), and produce a view of the 3D field.

- Calculate the magnetic field of a particular complicated current distribution, and produce an image of the field.

Over the next days I hope to have a chance to play around with some actual numerical E&M problems and see what I can come up with. And David, I promise that I will now go back to your assignments memo to read and consider it fully.