## Brief Bio and (PR)<sup>2</sup>: Problems & Pitches – Rants & Raves by Michael McLennan

#### Self Introduction



Michael McLennan is a Senior Research Scientist at Purdue University and Director of the HUBzero® Platform for Scientific Collaboration. HUBzero is an open source software platform used to build online collaboratories, including nanoHUB.org, NEES.org and more than 40 other sites supporting both education and research.

McLennan received a Ph.D. in 1990 from Purdue University, supported as an SRC Graduate Fellow, for his dissertation on dissipative quantum mechanical electron transport in semiconductor heterostructure devices. He spent 14 years working in industry at Bell Labs and Cadence Design

Systems, developing software for computer-aided design of integrated circuits. He created [incr Tcl], an object-oriented extension of the Tcl scripting language, which has been used by thousands of developers worldwide on projects ranging from the TiVo digital video recorder to the Mars Pathfinder. He coauthored two books, Effective Tcl/Tk Programming (Addison-Wesley, 1997) and Tcl/Tk Tools (O'Reilly Media, 1997). His latest project is the Rappture Toolkit, which accelerates the process of creating scientific tools for simulation and modeling.

#### **Publications**

- M. McLennan, R. Kennell, "HUBzero: A Platform for Dissemination and Collaboration in Computational Science and Engineering," *Computing in Science and Engineering*, 12(2):48-52 (2010).
- G. Klimeck, M. McLennan, S.P. Brophy, G.B. Adams III, and M.S. Lundstrom, "nanoHUB.org: Advancing Education and Research in Nanotechnology," *Computing in Science & Engineering*, 10(5):17-23 (2008).
- W. Qiao, M. McLennan, R. Kennell, DS Ebert, and G. Klimeck, "Hub-based simulation and graphics hardware accelerated visualization for nanotechnology applications," *IEEE Trans Vis Comput Graph.*, 12(5):1061-8 (2006).
- M. J. McLennan, Y. Lee and S. Datta "Voltage Drop in Mesoscopic Systems: A Numerical Study Using a Quantum Kinetic Equation," *Phys. Rev. B* 43, 13846 (1991).
- S. Datta and M. J. McLennan, "A Review of Quantum Transport in Ultrasmall Electronic Devices," Rep. Prog. Phys. 53, 1003 (1990).

Home page: <u>http://hubzero.org/members/1016</u> HUBzero: <u>http://hubzero.org/getstarted</u>

#### **General Questions**

#### 1) What are your main interests in attending the workshop?

I'm interested in new computational services that we could either integrate into HUBzero or offer to various communities through the various hubs that we operate.

#### 2) What are the tools or services you would like to share at the workshop?

I'd like to give others an introduction to the HUBzero software platform. HUBzero provides a unique blend of computation, data management, and social networking in a way that supports both research and

education. It's sort of an instant soup stock for cloud computing, data management, and online collaboration.

# 3) Please list three features or functions of your tools or services that are most important for the users.

- Content management system for simulation/modeling tools, with a safe environment for executing code. We don't trust the users who contribute the code nor the people who run it within any site.
- User interfaces that are easy to create via a drag-and-drop builder, easy to deploy online, and easy for users to visualize/analyze results. Our oldest hub, nanoHUB.org, has more than 260 simulation tools that are used by more than 12,000 people each year.
- Computational tasks can scale up to larger resources. HUBzero integrates with Globus, Condor, PBS, and other job submission protocols. It supports workflow management systems, such as the Pegasus workflow manager, so the click of a button can launch thousands of jobs.

### 4) What are the major concerns for the architect design of the tools and services?

We encourage separation of the graphical user interface (GUI) from the underlying simulation/modeling code, so that tools can be composed in workflows and sent off to remote systems for execution. HUBzero can host any code that runs in a Linux/X11 environment, and supports usage and integration at multiple levels—from the command line for experts to simple "calculator" tools for novices.

# 5) Are you aware of especially innovative approaches to plug-and-play feature where algorithms and plugins can be shared between different tools? If yes, please list down the approaches.

The Rappture toolkit within HUBzero standardizes the interface for the tools that use it. This integrates powerful visualization features and makes it easier for users to learn new tools, since the tools have a similar look and feel. Some people think of Rappture as a GUI builder, but it is really a data input/output standard and it encourages development of tools as reusable building blocks.

### 6) What are the challenges in developing the tools and services?

Encouraging tool builders to provide adequate support for their communities is a huge challenge. Developers need to provide better documentation, to answer questions from the community, and to stand behind their tools and fix bugs when they are reported. Many researchers think of these issues as an afterthought or as someone else's job. Advertising new hubs and building the user community is another huge challenge. Many projects underestimate the time it takes and the amount of work it requires.

### 7) Are you or your group working on any of these challenges? If yes, please explain.

We have created a support system within HUBzero that helps researchers respond to questions, fix bugs, integrate new features, and publish updated tools. We also help them attract and build a community of users. In a sense, we provide a bucket for water and we help lead the horses to water, but we cannot make them drink.

# 8) Does your development team contain volunteer developers? If yes, please explain how they are involved.

The content contributors on each hub are a volunteer community. We train them and encourage them, but in the end, they create the content for various hubs. Some developers also contribute at the infrastructure level by sending ideas and patches for the HUBzero code to our team at Purdue. We have a separate HUBzero Foundation to manage that activity.

### 9) What would you like to learn and achieve at the workshop?

I'd like to see what solutions others have devised to engage their communities, and look for software building blocks that could be integrated into the HUBzero system.