

Opennovation

Engineering Consulting with Open Source Tools



Opennovation, short for **open innovation**, specializes in solving engineering problems by means of open source analysis tools. Open source licensing allows **Opennovation** to deliver innovative solutions to meet client needs. The client may also use the resulting simulation software indefinitely on unlimited computers, making it more valuable than a one-time modeling contract.

For years, businesses have appreciated the benefits of open source software such as the Linux operating system kernel, Firefox web browser, MySQL and PostgreSQL databases, and OpenOffice suite. But open source does not only mean zero price. It also provides business with the freedom to service and maintain software tools, whether by in-house programmers or third parties, without being locked to a single vendor.

There is now a critical mass of open source software in the engineering modeling domain. **Opennovation** is uniquely qualified to bring the benefits of this software to businesses.

The core competencies of **Opennovation** are:

- **Transport Phenomena:** Building on years of design experience involving fluids and heat & mass transfer, **Opennovation** can often come to quick solutions to complex problems in this area. Principal Adam Powell is the founder of and primary contributor to the Transport Phenomena Archive on the Materials Digital Library.
- **Finite element and boundary element modeling:** **Opennovation** uses state-of-the-art open source parallel solvers and libraries to run complex finite element simulations in two or three dimensions, and can tailor its own in-house boundary element code called Julian to quickly solve complex problems in heat conduction, linear elastic mechanics, and electrochemistry.
- **Materials Selection and Behavior:** Materials are often the most complex part of a design, as their mechanical, thermal, electrical, and chemical behavior is often highly nonlinear and difficult to predict. Principal Adam Powell has expertise in materials selection for optimal mechanical and thermal behavior for a given application.

Though many companies can run straightforward simulations involving fluid flow or mechanical deformation, **Opennovation's** strength is its ability to develop new simulation strategies for complex multi-physics problems, and to implement algorithms published in science and engineering modeling literature. Examples of this are discussed below.

Opennovation Founder and Principal Dr. Adam C. Powell, IV is an engineering consultant with expertise in materials, transport, modeling, and high-performance computing. His consulting has included electrochemical smelting and refining, phase inversion processes used to make polymer membranes, and use of advanced materials in product design.

Dr. Powell's refereed publications address applications to polymer membranes, electrochemistry, solidification and casting defects, physical vapor deposition, solder wetting and solidification, and electron beam melting. He has developed open-source phase field, boundary element, and direct simulation Monte Carlo (DSMC) software that enjoys widespread use in research and education around the world. He is a co-author of a National Academies study on Integrated Computational Materials Engineering scheduled for publication in early 2008

Powell is nearly fluent in Japanese, including technical presentations, and has traveled to Japan frequently since participating in the MIT-Japan Program as an undergraduate. He maintains a desk as a Foreign Cooperative Researcher at the University of Tokyo International Research Center for Sustainable Materials.

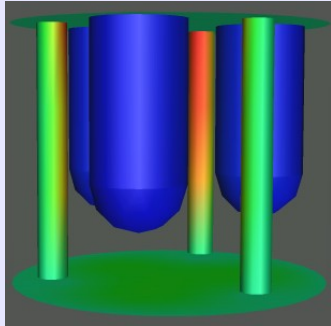
Powell holds twin Bachelors degrees from MIT in Materials Science and Engineering and Economics, and a Ph.D. in Materials Engineering also from MIT. After a postdoc position at NIST, he was a tenure track Professor at MIT, then a Managing Engineer at Veryst Engineering LLC, prior to founding **Opennovation**.

Opennovation Novel Simulation Implementations

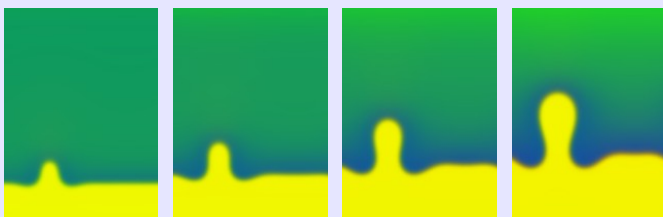
Electrochemistry Modeling

Modeling electrochemical processes presents several particularly difficult challenges, such as nonlinear boundary conditions and linking of phenomena at very different length scales. **Opennovation's** electrochemistry modeling capabilities range from macroscopic boundary element calculations of current density distribution, down to detailed modeling of micron-scale dendrites.

Macroscopic modeling predicts the distribution of current density at the electrodes. This enables an engineer to control the uniformity of metal plating and to determine whether some regions will plate with a rough instead of smooth surface. Such modeling is also crucial for the design of cathodic protection systems for corrosion prevention. Working with graduate student Rachel DeLucas, Powell adapted the Julian boundary element code to model solid oxide membrane (SOM) electrowinning of magnesium. The result shown above indicates uniform current density at the anodes (blue) and localized current density on the cathodes (red-green).



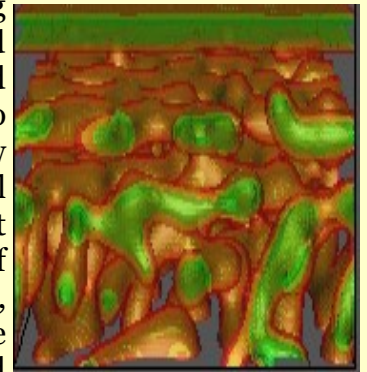
Microscopic electrochemistry models are helpful for understanding the formation of rough surfaces during plating. Working with graduate students Wanida Pongsaksawad and David Dussault, Powell adapted a solidification methodology called Phase Field to calculate the shape of dendrites formed by electrowinning of metals. This methodology is also useful for designing AC waveforms for various objectives, such as fast plating without roughness, surfaces with controlled dendrite morphology, or metal powder production.



Polymer Membranes

Most polymer membranes for water filtration are made by a phase inversion process, such as immersion precipitation, solvent evaporation, or thermal-induced phase separation. These processes can form a wide variety of membrane structures; membrane structure in turn determines properties such as permeability, selectivity and strength.

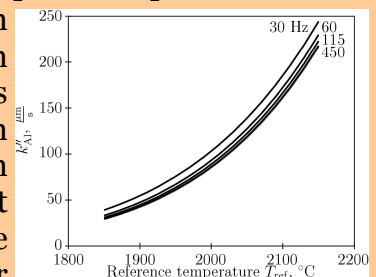
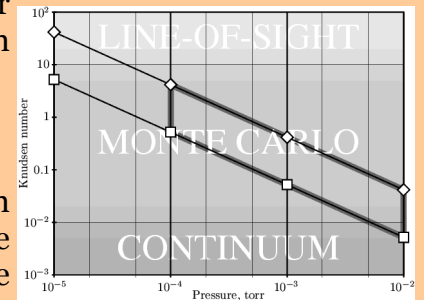
Unfortunately, the mechanisms of structure formation have been largely unknown, making membrane engineering a process of trial and error. Powell and graduate student Bo Zhou developed a new Phase Field model which can predict many aspects of membrane structure, such as pore structure and presence and thickness of a dense skin layer.



Evaporation Processes

The performance of physical vapor deposition processes and hearth melting of metals depend on vapor transport and often multicomponent evaporation.

Opennovation's Direct Simulation Monte Carlo code can predict the extent of vapor plume focusing in evaporation processes. And its model of electron beam evaporation can predict the dynamics of alloy composition due to differences in constituent element vapor pressures. These can be used together to model deposition of thin films of alloys and multicomponent ceramics.



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