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# Chemistry Pathways Report

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# Chemistry Pathways – Past and Present

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- CCCE Workshops (NCSI & SC sponsored)
  - One-week workshops; Three levels:
    - Introduction to Computational Chemistry Education
      - Some Molecular Modeling, More Visualization
        - » Tools: Excel, Vensim PLE, CSERD
    - Computational Chemistry: Molecular Modeling
      - Mostly Molecular Modeling, Some Visualization
        - » Tools: WebMO, Mathcad/Mathematica
    - Advanced Chemical Computation
      - Module preparation and adaptation
      - In-depth applications, Biochemistry, Drug Design



# Chemistry Pathways - Past and Present

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- One-half to Two and one-half day workshops
  - College faculty & Graduate students
  - High School teachers
    - Local American Chemistry Society meetings
    - Regional ACS Meetings
    - By invitation (Univ. of Pittsburgh, Sigma Xi)
- Institute for Chemistry Literacy through Computational Science (ICLCS)
  - Two-week Illinois High School teacher workshops



# Materials Collection: CCCE

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- <http://www.computationalscience.org/ccce/>
- To Do's
  - Collect finished modules from past participants and add to the above site
    - College and High School collections
  - Add voiceovers to lectures and screen-capture video for software instructions
  - Provide links to additional resources
  - Add WebMO instructions to the matrix
    - Include multiprocessor instructions



# $\Delta(\text{Workshop}) / \Delta(\text{time})$

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- 2003 – 2005
  - Variety of MM software provided on each machine
  - Limited by machine CPU speed and memory
- 2005 – Present
  - More use of remote servers/clusters via WebMO
  - <http://bobsced.cluster.earlham.edu/cgi-bin/login.cgi>
  - Ability to perform parallel jobs
  - New installs
    - Easier deployment, less cost, wider access, more simple maintenance and upgrades

# WebMO

- Web-based GUI
- Open source and commercial computational engines can be used:

## Choose Computational Engine

The screenshot displays the 'Choose Computational Engine' web interface. On the left, a sidebar shows the user's status as 'guest' and 'webmo', with a timer at '1:00' and '0 jobs' remaining. The progress bar indicates the current step is 'Choose engine'. Below the progress bar, there are links for 'Job manager', 'Build molecule', 'Choose engine', 'Job options', 'Submit job', and 'Help'. The main area features a table of computational engines with radio buttons for selection. The 'Gamess' engine is selected. Below the table, a 'Select Server' dropdown menu is set to 'buchner.chem.hope.edu'. Navigation arrows are visible at the bottom of the main area.

Engine	Description
<input checked="" type="radio"/> Gamess	Ab initio and semi-empirical calculations
<input type="radio"/> Gaussian	Ab initio and semi-empirical calculations
<input type="radio"/> Molpro	Ab initio calculations
<input type="radio"/> Mopac	Semi-empirical calculations
<input type="radio"/> NWChem	Ab initio calculations
<input type="radio"/> QChem	Ab initio calculations
<input type="radio"/> Tinker	Molecular mechanics calculations

Select Server: buchner.chem.hope.edu

# Chemistry Pathways - The Future

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- Better Publicity = Higher workshop attendance
- Hardware: Additional Cores/Processors
  - Software will have to catch up to Hardware
    - Will enable more biochemical modeling
- What are others doing?
- CCLI Phase II Proposal
  - Test educational effectiveness in chemistry
- Petascale machine install at NCSA-UIUC
  - Be prepared to take advantage of this resource