The How to Give a Talk

Christopher J. Cramer

University of Minnesota, March 6, 2014
What’s at Stake When You Give a Talk?

Everything!

A job candidate lives or dies in that one hour
In my personal experience, 75% of all talks are a waste of my time

Instead of fearing the risk, embrace the opportunity for reward…
Before You Start:

• Know your audience (ask if unsure); pitch general or targeted

• Know your time limit (ask if unsure)

• Know your available technology (ask — ok, you get it…)

• What impression are you trying to make?

• What are you wearing? You’re *performing*; costume matters

• Practiced? (It helps until it hurts)
The Title Slide

Engaging, Professional — not too long or too technical a title, please — same if you were asked for an abstract

Christopher J. Cramer (and co-workers — thank early)

University of Minnesota, March 20, 2012
My Secrets After 20 Years

• A good talk is a story-telling performance. Imagine telling a story to your favorite 7-year old, and shoot for *that style*.

• Less is more. Your audience will give you far more credit for a shorter story, *that they really felt like they understood*, than they will for a turgid trilogy that just blew by them.

• It is entirely likely that you know more about your science than anyone else in the room. Bring them up to speed in a methodical and informative manner. Teach to Jethro!

• Never run long. *Never*. It’s disrespectful, and it illustrates your complete inability to plan. If you have to cut material, then cut it — even on the fly. (I assume 2.5 minutes per slide — get to know your own number with practice.)
Organization After That Title Slide

• An outline? Why? Are you expecting someone to leave?

• Big picture, introductory material. Why the hell should I, a person outside your research group, give a damn about what you’re about to tell me? Why might a funding agency, or humanity in general, care?

• Any really critical discussion of instruments, techniques, spectral interpretation, or other non-generally-well-known concepts that will permeate your talk if and only if you can actually get that across in a modest time window

• Narrative results. Interim conclusions (if helpful). More results. More conclusions. Circle back to your big picture. What are the remaining open questions? What’s next?
Organization After That Title Slide

• Big picture, introductory material. Students in particular like this — they may not remember exactly what you were doing, but they’ll remember that they learned something new from a big picture perspective.
A One-Slide Summary of Computational Chemistry
(aka: theoretical chemistry, molecular modeling)

Why do it?

- to rationalize experiment
- confirming other data
- to improve the design of the next experiment
- prioritizing multiple experiments
- to (gasp) replace experiment

Personal aside: computation and waste disposal—guess which keeps getting exponentially cheaper and which keeps getting exponentially more expensive...
Dioxygen Activation at Monocopper Sites

Dopamine β-Monooxygenase (DβM)

\[
\text{Dopamine} \quad \text{HS} \quad \text{HR} \quad \text{NH}_2 \quad 2e^- + 2H^+ + O_2 \quad \text{- H}_2\text{O} \quad \text{Norepinephrine} \quad \text{HS} \quad \text{OH} \quad \text{NH}_2
\]

Peptidylglycine α-Hydroxylating Monooxygenase (PHM)

\[
\text{Peptide} \quad \text{NH} \quad \text{C} \quad \text{COOH} \quad 2e^- + 2H^+ + O_2 \quad \text{- H}_2\text{O} \quad \text{Peptide} \quad \text{NH} \quad \text{C} \quad \text{COOH} \quad \text{HO} \quad \text{HR}
\]
Conversion of Solar Energy to Green Fuel

Schematic of the Dye-Sensitized Solar Cell

\[ 2\text{H}_2\text{O} \xrightarrow{\text{solar energy}} \text{O}_2 + \text{H}_2 \]
What Do We Predict with SMx Solvation Models?

By combining these, we also calculate solubility.

Have also extended to:
• Interface adsorption
• Membrane permeability
Organization After Those Introductory Slides

• Any really critical discussion of instruments, techniques, spectral interpretation, or other non-generally-well-known concepts that will permeate your talk *if and only if* you can actually get that across in a modest time window
Potential Energy Surface Perspective

Phase partitioning from separation between the surfaces themselves

Equilibrium constants from differences in energy of local minima

Rate constants from differences in energy of connected local minima and saddle points
SMx Bulk Electrostatic Effects

Generalized Born (GB) equation

\[ G_P = -\frac{1}{2} \left( 1 - \frac{1}{\varepsilon} \right)^{atoms} \sum_{kk'} q_k \gamma_{kk'} q_{k'} \]

Polarized Continuum Model (PCM) equation

\[ G_P = -\frac{1}{2} \left( \langle \Psi | V_{RF} | \Psi \rangle + \sum_k Z_k V_{RF} \right) \]

Reaction field—usually

\[ V_{RF}(r) = \sum_{k'} \frac{q_{k'}}{|r - r_{k'}|} \]

Limiting behaviors...

- \( r_{kk'} \gg 0 \)
  \[ G_P = -\frac{1}{2} \left( 1 - \frac{1}{\varepsilon} \right) \frac{q_k q_{k'}}{r_{kk'}} \]
  
  **Coulomb’s Law**
  
  \( 1/2 (-\text{gas} + \text{solution}) \)

- \( r_{kk'} = 0 \)
  \[ G_P = -\frac{1}{2} \left( 1 - \frac{1}{\varepsilon} \right) \frac{q_k^2}{\alpha_k} \]

  **Born’s Equation**

  monatomic ion
Pet Peeve

• If you can’t explain an equation fully — every term — then leave it out. If you just have to have it, devote the necessary time to explain it. You’ll lose half the audience with your first equation that flashes by with an inadequate explanation. Your job is to make the equation seem intuitive.

The same holds true for reagent acronyms in synthetic schemes… Spectra with unexplained features… etc.

In sum, if you put it on the slide, explain it. If you aren’t going to explain it, why did you put it on the slide? To show off how smart you are? Bad move…
\[
\frac{\partial q_k}{\partial P_{\mu \nu}} = \delta_{\mu \nu} \left[ \delta_{k(k(\mu)} (-1 - B_k c_k) + \left(1 - \delta_{k(k(\mu))} \right) B_{k(k(\mu))} c_{k(\mu)} \right] \\
\left(1 - \delta_{k(k(\mu))} \right) \left(1 - \delta_{k(k(\nu))} \right) \left[ - B_{k(k(\mu))} \left( \delta_{k(k(\mu))} H_{\mu \nu} P_{\mu \nu} d_{H_k(\nu)} + \delta_{k(\mu)O} P_{\mu \nu} d_{O_k(\nu)} \right) \right] \\
+ \left(1 - \delta_{k(\mu)} k_{(\nu)} \right) \left[ + \left( \delta_{k(k(\mu))} + \delta_{k(k(\nu))} \right) \right] \\
+ \left( \delta_{k(k(\mu))} + \delta_{k(k(\nu))} \right) \left[ P_{\mu \nu} \left[ c_k q_k^{(0)} + (1 - \delta_{kH}) d_k + \delta_{kH} \sum_{k' \neq k} B_{k(k)} d_{H_k(k')} + \delta_{kO} \sum_{k' \neq k} B_{k(k)} d_{O_k(k')} \right] \right] \\
+ \left( \delta_{k(k(\mu))} + \delta_{k(k(\nu))} \right) \left[ \right]
\]
Some Technical Things

• You’ve already seen how I like bulleted text.

• Slide backgrounds: Keep ‘em simple. Unless you’re selling worthless stocks, you want your audience focused on your slides’ contents, not some fabulous wallpaper that you also proudly use on your Twitter homepage.

• If you do want to appear and disappear things (which can definitely be a useful way to focus your audience’s attention!), keep it simple: on/off, or maybe grayout in certain instances. Avoid garish spinning, sliding, exploding, etc.

• Font sizes. Never, ever less than 14 pt on a landscape slide, and that small only for citations, for example. If it won’t all fit on one slide, you’ve got too much on the slide…
$\text{CuO}_2^+$

$\Delta E_{\text{rel}}$ to end-on triplet

**bold line** = restricted DFT

**thin line** = broken-symmetry spin-purified DFT

- side-on singlet
- side-on triplet
- end-on singlet

$k$-cal/mol
Tabular data

• Is there a number you don’t plan to mention? Then why did you display it?

• Bigger fonts are better.

• Highlight the most important data where warranted.

• Keep borders clean and simple
**SM8 Performance (OK table)**

*Mean unsigned errors (kcal/mol) for SM8 and some other popular continuum solvation models*

<table>
<thead>
<tr>
<th>Solute class</th>
<th>Data $N$</th>
<th>SM8 $G03/UA0$</th>
<th>IEF-PCM $G03/UA0$</th>
<th>C-PCM $GAMESS$</th>
<th>PB $Jaguar$</th>
<th>All equal to mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>aqueous neutrals</td>
<td>274</td>
<td>0.5</td>
<td>4.9</td>
<td>1.6</td>
<td>0.9</td>
<td>2.7</td>
</tr>
<tr>
<td>nonaq. neutrals</td>
<td>666</td>
<td>0.6</td>
<td>6.0</td>
<td>2.8</td>
<td>2.3</td>
<td>1.5</td>
</tr>
<tr>
<td>aqueous ions</td>
<td>112</td>
<td>3.2</td>
<td>12.4</td>
<td>8.4</td>
<td>4.0</td>
<td>8.6</td>
</tr>
<tr>
<td>nonaqueous ions</td>
<td>220</td>
<td>4.9</td>
<td>8.4</td>
<td>8.4</td>
<td>8.1</td>
<td>8.6</td>
</tr>
</tbody>
</table>


## SM8 Performance (Poor table)

<table>
<thead>
<tr>
<th>compound</th>
<th>SM8</th>
<th>exp</th>
</tr>
</thead>
<tbody>
<tr>
<td>uracil</td>
<td>–16.76</td>
<td>–16.59 ± 0.28</td>
</tr>
<tr>
<td>5-bromouracil</td>
<td>–16.39</td>
<td>–18.17 ± 0.55</td>
</tr>
<tr>
<td>5-chlorouracil</td>
<td>–16.59</td>
<td>–17.74 ± 0.78</td>
</tr>
<tr>
<td>5-fluorouracil</td>
<td>–17.38</td>
<td>–16.92 ± 0.88</td>
</tr>
<tr>
<td>5-trifluoromethyluracil</td>
<td>–16.52</td>
<td>–15.46 ± 0.16</td>
</tr>
<tr>
<td>6-chlorouracil</td>
<td>–14.24</td>
<td>–15.83 ± 1.22</td>
</tr>
<tr>
<td>cyanuric acid</td>
<td>–20.32</td>
<td>–18.26 ± 0.27</td>
</tr>
<tr>
<td>caffeine</td>
<td>–11.90</td>
<td>–12.64 ± 0.74</td>
</tr>
<tr>
<td>methyl paraben</td>
<td>–9.85</td>
<td>–9.51 ± 0.26</td>
</tr>
<tr>
<td>ethyl paraben</td>
<td>–9.50</td>
<td>–9.20 ± 0.30</td>
</tr>
<tr>
<td>propyl paraben</td>
<td>–9.24</td>
<td>–9.37 ± 0.22</td>
</tr>
<tr>
<td>butyl paraben</td>
<td>–8.42</td>
<td>–8.72 ± 0.27</td>
</tr>
<tr>
<td>acetylsalicylic acid</td>
<td>–11.93</td>
<td>–9.94 ± 0.18</td>
</tr>
<tr>
<td>diflunisal</td>
<td>–13.96</td>
<td>–9.40 ± 0.20</td>
</tr>
<tr>
<td>flurbiprofen</td>
<td>–9.03</td>
<td>–8.42 ± 0.16</td>
</tr>
<tr>
<td>ibuprofen</td>
<td>–6.88</td>
<td>–7.00 ± 0.64</td>
</tr>
<tr>
<td>ketoprofen</td>
<td>–12.56</td>
<td>–10.78 ± 0.18</td>
</tr>
<tr>
<td>naproxfen</td>
<td>–10.90</td>
<td>–10.21 ± 0.18</td>
</tr>
<tr>
<td>phthalimide</td>
<td>–11.99</td>
<td>–9.61 ± 0.50</td>
</tr>
<tr>
<td>sulfonamide</td>
<td>–13.26</td>
<td>–8.61 ± 0.31</td>
</tr>
<tr>
<td><strong>D-glucose</strong></td>
<td><strong>–25.29</strong></td>
<td><strong>–25.47 ± 0.22</strong></td>
</tr>
<tr>
<td><strong>D-xylose</strong></td>
<td><strong>–21.71</strong></td>
<td><strong>–20.52 ± 0.27</strong></td>
</tr>
</tbody>
</table>

Adding More Waters \((\text{Best Table})\)

**Experimental \(pK_a\)'s**

\[
\begin{align*}
\text{H}_2\text{CO}_3 & \quad \text{HCO}_3^- & \quad \text{CO}_3^{2-} \\
pK_{a1} = 6.4 & \quad \text{pK}_{a2} = 10.3 \\
\end{align*}
\]

**Calculated \(pK_a\)'s**

<table>
<thead>
<tr>
<th>No. H(_2)O</th>
<th>(pK_{a1})</th>
<th>(pK_{a2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.6</td>
<td>1.6</td>
</tr>
<tr>
<td>1</td>
<td>1.3</td>
<td>5.0</td>
</tr>
<tr>
<td>2</td>
<td>2.3</td>
<td>7.8</td>
</tr>
<tr>
<td>3</td>
<td>4.2</td>
<td>9.0</td>
</tr>
</tbody>
</table>

Adding explicit water molecules improves the accuracy of the calculation.
Known LCuO₂ Models—Substantial Diversity

Ensure all structures are big enough to be easily seen in the back row; be consistent in how you draw all structures (bond lengths, fonts)

PHM precatalytic complex
\( r_{O-O} = 1.23 \text{ Å} \)
ground state

Schindler et al.
\( r_{O-O} = 1.28 \text{ Å} \)
ground state triplet

Karlin et al.
\( r_{O-O} = ? \)
ground state

Kitajima et al.
\( r_{O-O} = [1.33] \text{ Å} \)
ground state singlet

Tolman et al.
\( r_{O-O} = 1.39 \text{ Å} \)
ground state singlet

If you need to show 3D structures, consider having them rotate (looped) to improve perspective
A Host-Guest System That Needs Animation
Oxidation State of Ru?

Triplet SOMOs

$L_4$Ru

 colors are good (within limits)
highlight boxes are very good to organize slides

$\pi$ hybridization of octahedral Ru$^{II}$
d orbitals with 2 neutral O atoms
Stop-flow Kinetics for Oxygenation

Do your best to get all related data, concepts, conclusions, on single slides

\[
\frac{\partial [L^1\text{CuO}_2]}{\partial t} = k_A[L^1\text{Cu(MeCN)}][O_2] + k_B[L^1\text{Cu(MeCN)}]
\]
A One-Slide Summary of Computational Chemistry
(aka: theoretical chemistry, molecular modeling)

Why do it?
- to rationalize experiment
- confirming other data
- prioritizing multiple experiments
- to improve the design of the next experiment
- validated model can now be used to design improved catalysts in silico prior to synthetic efforts
- to (gasp) replace experiment
- explained ambiguities, corrected errors

Personal aside: computation and waste disposal—guess which keeps getting exponentially cheaper and which keeps getting exponentially more expensive...

circling back; conclusions don’t have to be bulleted text
Acknowledgments

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Prof. Piotr Piecuch (MSU)
Prof. Bill Tolman (Minnesota)
Dirty Little Secret

• Every rule I’ve just laid down, I’ve felt free to violate at one time or another. *But*, only when I’ve believed the payoff to outweigh the unprofessionalism.

THANKS!!

• Questions welcome