Open Structure:
Ontology Repair Plan based on Atomic Modeling

Jos Lehmann
joint work with Alan Bundy and Michael Chan

School of Informatics, University of Edinburgh

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Outline

1. Overview GALILEO Project
   - Ontology Evolution in Physics

2. A Case Study in Atomic Modeling
   - From Thomson’s to Rutherford’s atom

3. Ontology Repair Plan based on Case Study
   - Open Structure

4. Discussion
   - Future work
Aim: solving contradictions between multiple ontologies.

- Canonical case: contradictions in physics between theoretical expectations and experimental observations.

Main results: Ontology Repair Plans (ORPs).

- Trigger: detects contradiction between ontologies.
- Repair: changes ontology axioms or signature.
- Create New Axioms: propagates changes as needed.

Methodology: turn case studies in physics history into ORPs.

- Extract ORP’s conceptual backbone from case study.
- Represent ORP in higher-order logic.
- Implement ORP (λProlog and beyond).

Some ORPs and their state of development.

- Developed and tested: Where’s My Stuff?, Inconstancy, Unite.
- Being tested: Open Structure, Close Structure.
- Under development: Unify.
Thomson’s atom (1904) and Rutherford’s atom (1911)

- 11 electron atom and 15 electron atom.
- Black dots and circumferences represent negative charges and their orbits/rings.
- Red circles represent positive charge (more intense where darker).
- Note that Rutherford’s atom’s structure is monotonic: Thomson’s atom’s configuration changes when electrons are added, Rutherford’s atom’s configuration is stable.
Rutherford’s scattering apparatus (1898-1911)

- R, fixed source of $\alpha$-particles (double positive charges).
- D, collimating diaphragm.
- F, fixed foil.
- S, screen.
- M, microscope.
- Chamber is evacuated and can be rotated around F.
- Original image in (Geiger, 1913), downloaded from. [http://galileo.phys.virginia.edu](http://galileo.phys.virginia.edu)
Expected vs observed scattering

- Red spots and lines are $\alpha$-particles and their paths.
- Half-dashed thin red lines are ideal undeflected paths.
- $b$’s and $-b$’s are impact parameters ($b = 0$ for third particle).
- $r$’s are distances between a point of the atom’s electric field and the atom’s center.
- $R$ is the atom’s radius.
- $th$’s are scattering angles.
- Expected scattering is minimal.
- Observed scattering is minimal, large or a complete rebound.
The nucleus explains the difference between expectations and observations.

The nucleus entails different deflection functions:

\[ \theta(b)_{\text{Thomson}} \text{ and } \theta(b)_{\text{Rutherford}} \] calculate different deflection angles for same \( b \)'s.

The nucleus also entails different scattering potential functions:

\[ V(r)_{\text{Thomson}} \text{ and } V(r)_{\text{Rutherford}} \] calculate different amounts of work exerted by positive electric fields when deflecting incident particles at same distance \( r \).
Scattering potential functions for different structures

\[ V(r)_{\text{Thomson}} = \begin{cases} 
\frac{Q_A Q_B}{4\pi\epsilon_0} \frac{1}{r} & R \leq r \\
\frac{Q_A Q_B}{4\pi\epsilon_0} \frac{1}{2R^3} (3R^2 - r^2) & 0 \leq r \leq R 
\end{cases} \]

\[ V(r)_{\text{Rutherford}} = \frac{Q_A Q_B}{4\pi\epsilon_0} \frac{1}{r} \]

where \( Q_A \) is the charge of incident particle, \( Q_B \) is the charge of the target atom, \( 1/4\pi\epsilon_0 \) is the Coulomb constant, \( r \) is the distance between the incident particle and the centre of the target atom, \( R \) is the radius of the target atom.

- \( V(r)_{\text{Thomson}} \) is both non-Coulombic (i.e. for values of \( r \) lower than the atom’s radius \( R \), the potential is directly proportional to \( r \)) and Coulombic (i.e. for values of \( r \) higher than \( R \), the potential is inversely proportional to \( r \)).
- \( V(r)_{\text{Rutherford}} \) is only Coulombic (\( R \) needs not to be considered).
- Formulae taken from (Zoli, 1998)


Evolution of $V(r)$ by existing ORPs

\[
V(r)_{\text{Thomson}} = \begin{cases} 
\frac{Q_A Q_B}{4 \pi \epsilon_0} \frac{1}{r} & R \leq r \\
\frac{Q_A Q_B}{4 \pi \epsilon_0} \frac{1}{2R^3} (3R^2 - r^2) & 0 \leq r \leq R
\end{cases}
\]

\[
V(r)_{\text{Rutherford}} = \frac{Q_A Q_B}{4 \pi \epsilon_0} \frac{1}{r}
\]

- **Where is my stuff?** would stick to Thomson’s atomic structure by increasing $Q_A$ and yielding evolution $V(r) \coloneqq V(r)_{\text{vis}} + V(r)_{\text{invis}}$. Problem: how would the additional charge be distributed wrt $R$?
- **Unite**, the inverse of Where is my stuff?, would not be able to let $V(r)$ evolve.
- **Incons** too would stick to Thomson’s atomic structure and let $V(r)$ evolve in such a way that the Coulomb constant $1/4 \pi \epsilon_0$ would depend on distance $r$ from the center of atom. This would yield a very complicated structure.
- **Need for an ORP that handles structural evolution as such**, rather than by pivoting on quantities.
- Formulae taken from (Zoli, 1998)
Open Structure ORP: Trigger

**Trigger**: $O_t \vdash d_4 > d_3 \geq cop \geq d_2 > d_1 \land$

$$((stuff(d_2) > stuff(d_1) \land stuff(d_3) > stuff(d_4)) \lor$$

$$(stuff(d_1) > stuff(d_2) \land stuff(d_4) > stuff(d_3))).$$

,$O_s \vdash \forall d, d' : \delta. \ d' > d \rightarrow stuff(d) > stuff(d').$

- **stuff** represents function subject to evolution (V is stuff).
- **stuff** ranges over a type $\delta$ of d’s (like V ranges over the type dis of distances r’s).
- **stuff**’s domain contains a cut-off point $cop$ (like V’s domain contains $R$).
- $K$ is constant (like all other quantities remain constant throughout V’s evolution).

Two cases of contradiction:

**crested* vs open structure** In $O_t$, for all arguments below cut-off point, value of **stuff** is directly proportional to argument, inversely proportional otherwise. In $O_s$ value of **stuff** is always inversely proportional to argument.

**trenched* vs open structure** In $O_t$, for all arguments below cut-off point, value of **stuff** is inversely proportional to the argument while, directly proportional otherwise. $O_s$ is the same as in the first case above.

*tentative term
Open Structure: \( \nu(stuff) ::= \lambda d : \delta. K/d. \)

Create New Axioms: 
\[
Ax(\nu(O_t)) ::= Ax(O_t) \setminus \{stuf::= \lambda d : \delta. (cop > d \land Kd) \lor K/d\} \cup \{\nu(stuff) ::= \lambda d : \delta. K/d\}. 
\]
\[
Ax(\nu(O_s)) ::= Ax(O_s) \setminus \{stuf::= \lambda cop, d : \delta. (cop > d \land Kd) \lor K/d\} \cup \{\nu(stuff) ::= \lambda d : \delta. K/d\}. 
\]

Contradiction always repaired according to what dictated by \( O_s \).
Application of Open Structure

**Substitution**:
\[
\left\{ \frac{Q_A Q_B}{4\pi\varepsilon_0}, V/stuff, d_i/r_i, \text{cop}/R \right\}
\]

**Trigger**:
\[
O_t \vdash r_4 > r_3 \geq R \geq r_2 > r_1 \land
((V(r_2) > V(r_1) \land V(r_3) > V(r_4))
O_s \vdash \forall r, r': \text{dis. } r' > r \rightarrow V(r) > V(r').
\]

**New Axioms**:
\[
\begin{align*}
\text{Ax}(\nu(O_t)) & := \text{Ax}(O_t) \setminus \\
& \left\{ V := \lambda r : \text{dis. } (R > r \land Kr) \lor K/r \right\} \cup \\
& \left\{ \nu(V) := \lambda r : \text{dis. } K/r \right\}.
\end{align*}
\]
\[
\begin{align*}
\text{Ax}(\nu(O_s)) & := \text{Ax}(O_s) \setminus \\
& \left\{ V := \lambda r : \text{dis. } (R > r \land Kr) \lor K/r \right\} \cup \\
& \left\{ \nu(V) := \lambda r : \text{dis. } K/r \right\}.
\end{align*}
\]
Future work

- Find other cases for application of Open Structure.
- Interpret its inverse, Close Structure, and find cases of application.
- Alternative treatment of Thomson vs Rutherford case study: modeling the evolution between the two atoms in terms of their different deflection functions.