VRG – Supporting Information

Communications excerpts with a university professor. An early cut at a database SQL schema to hold PDB protein data as an attachment (sample follows below, with time stamp and labeled "virion") shared with Professor Ng. The shared SQL schema shows usage of the name VIRION connected with our work. *In this scenario, software was "transported" externally as an open source (free) share of a SQL schema related to the Rutgers Protein Data Bank (PDB) data files. This is a form of "downloadable software" for Class 09, in the spirit of a dual licensing scheme that differentiates academic (free) and commercial usage (fee).*

From: Paul Conlon [mailto:pconlon@rochester.rr.com]
Sent: Tuesday, February 24, 2015 9:48 PM
To: 'hng@hawaii.edu'
Subject: RE: Hello from freezing New York!

One of the first cuts. I am changing things around....and nothing will refine your work like importing thousands of files ☺ It is just work....to chug thru it...and to use tools/tricks to move it along.

I didn't say this before, but I believe having this database and the data in it....is the way to learn chemistry. Life is the master chemist....maybe the order isn't right for teaching. Learn chemistry by getting this data, calculating bond lengths, and angles...use actual enzymes to learn about such reactions...learning physics from the interaction of molecular forces (if I didn't say this...I believe the jitter of molecules is only partly thermo...I think there is a servomechanism at play...with varying phases of "lock-in"). In a nutshell, the proposal is to integrate learning of this much the way I intend to. Comp sci too with graph theory and combinatorics algorithms....and group theory. Basically a holistic learning program based on real life data with real life problems.

/paul

From: Ho Leung Ng [mailto:hng@hawaii.edu]
Sent: Tuesday, February 24, 2015 1:36 AM
To: Paul
Subject: Re: Hello from freezing New York!

Hi Paul,

I agree with many of your points. Much scientific software is written by people like me, scientists who know how to use computers but lacking formal training in software engineering. Resources and incentives are not there from funding agencies and academic bodies to develop and maintain good software. I am intrigued by the possibilities of crowd sourcing scientific research, so we can take advantage of the many talented minds out there, and provide educational opportunities to students and learners. Imagine if we could duplicate the success of Linus Torvalds and Linux throughout other fields of science!

Our current computational projects involve 1) development of methods to locate hydrogen atoms from crystal structures, 2) using docking and modeling to develop drugs against cancer and immunology drug targets, and 3) modeling and investigating the effects of dynamics and flexibility in fluorescent proteins.

Outside of the projects themselves, I am interested in developing a platform for crowdsourcing, matching researchers (professionals, amateurs, and students) with like minded interests with projects.

Do any of these sound interesting to you? Would love to hear more about the state of your current project too.

Aloha,
Ho

Ho Leung Ng
University of Hawaii at Manoa
Assistant Professor, Department of Chemistry
hng@hawaii.edu

The **VRG** software developers do not have an academic background in biophysics/biochemistry. Professor Ng has been extremely helpful as we develop our software, answering our questions and explaining many things. He will receive an updated and highly functional prototype database, targeted by end of 2019. It will be suitable for scientific research. Another larger database prototype has over 1.5 million 3D protein atom coordinate database records.

PDB (Protein Data Bank) files from Rutgers University have a published form. We have downloaded nearly 100K files and have worked on creating a full database version.

```
--
-- PostgreSQL database dump
--

-- Dumped from database version 9.2.4
-- Dumped by pg_dump version 9.3.1
-- Started on 2014-02-08 19:39:28

SET statement_timeout = 0;
SET lock_timeout = 0;
SET client_encoding = 'UTF8';
SET standard_conforming_strings = on;
SET check_function_bodies = false;
SET client_min_messages = warning;

DROP DATABASE virion;
--
-- TOC entry 3544 (class 1262 OID 38254)
-- Name: virion; Type: DATABASE; Schema: -; Owner: virion
--

CREATE DATABASE virion WITH TEMPLATE = template0 ENCODING = 'UTF8' LC_COLLATE = 'English_United States.1252'
LC_CTYPE = 'English_United States.1252' TABLESPACE = virion;


ALTER DATABASE virion OWNER TO virion;

\connect virion

SET statement_timeout = 0;
SET lock_timeout = 0;
SET client_encoding = 'UTF8';
SET standard_conforming_strings = on;
SET check_function_bodies = false;
SET client_min_messages = warning;

--
-- TOC entry 6 (class 2615 OID 38255)
-- Name: pdb; Type: SCHEMA; Schema: -; Owner: virion
--

CREATE SCHEMA pdb;


ALTER SCHEMA pdb OWNER TO virion;

--
-- TOC entry 507 (class 3079 OID 11727)
-- Name: plpgsql; Type: EXTENSION; Schema: -; Owner:
--

CREATE EXTENSION IF NOT EXISTS plpgsql WITH SCHEMA pg_catalog;


--
-- TOC entry 3545 (class 0 OID 0)
-- Dependencies: 507
-- Name: EXTENSION plpgsql; Type: COMMENT; Schema: -; Owner:
--

COMMENT ON EXTENSION plpgsql IS 'PL/pgSQL procedural language';


SET search_path = pdb, pg_catalog;

SET default_tablespace = '';

SET default_with_oids = false;




--
-- TOC entry 168 (class 1259 OID 38256)
-- Name: atom_site; Type: TABLE; Schema: pdb; Owner: virion; Tablespace:
```

```
--

CREATE TABLE atom_site (
    id character varying(255),
    b_equiv_geom_mean double precision,
    b_equiv_geom_mean_esd double precision,
    b_iso_or_equiv double precision,
    b_iso_or_equiv_esd double precision,
    cartn_x double precision,
    cartn_x_esd double precision,
    cartn_y double precision,
    cartn_y_esd double precision,
    cartn_z double precision,
    cartn_z_esd double precision,
    u_equiv_geom_mean double precision,
    u_equiv_geom_mean_esd double precision,
    u_iso_or_equiv double precision,
    u_iso_or_equiv_esd double precision,
    wyckoff_symbol character varying(255),
    adp_type character varying(255),
    aniso_b11 double precision,
    aniso_b11_esd double precision,
    aniso_b12 double precision,
    aniso_b12_esd double precision,
    aniso_b13 double precision,
    aniso_b13_esd double precision,
    aniso_b22 double precision,
    aniso_b22_esd double precision,
    aniso_b23 double precision,
    aniso_b23_esd double precision,
    aniso_b33 double precision,
    aniso_b33_esd double precision,
    aniso_u11 double precision,
    aniso_u11_esd double precision,
    aniso_u12 double precision,
    aniso_u12_esd double precision,
    aniso_u13 double precision,
    aniso_u13_esd double precision,
    aniso_u22 double precision,
    aniso_u22_esd double precision,
    aniso_u23 double precision,
    aniso_u23_esd double precision,
    aniso_u33 double precision,
    aniso_u33_esd double precision,
    aniso_ratio double precision,
    attached_hydrogens integer,
    auth_asym_id character varying(255),
    auth_atom_id character varying(255),
    auth_comp_id character varying(255),
    auth_seq_id character varying(255),
    calc_attached_atom character varying(255),
    calc_flag character varying(255),
    chemical_conn_number integer,
    constraints character varying(255),
    details character varying(255),
    disorder_assembly character varying(255),
    disorder_group character varying(255),
    footnote_id character varying(255),
    fract_x double precision,
    fract_x_esd double precision,
    fract_y double precision,
    fract_y_esd double precision,
    fract_z double precision,
    fract_z_esd double precision,
    group_pdb character varying(255),
    label_alt_id character varying(255),
    label_asym_id character varying(255),
    label_atom_id character varying(255),
    label_comp_id character varying(255),
    label_entity_id character varying(255),
    label_seq_id integer,
    occupancy double precision,
    occupancy_esd double precision,
    pdbx_pdb_atom_name character varying(255),
    pdbx_pdb_ins_code character varying(255),
    pdbx_pdb_model_num integer,
    pdbx_pdb_residue_name character varying(255),
    pdbx_pdb_residue_no character varying(255),
    pdbx_pdb_strand_id character varying(255),
```

```
      pdbx_auth_alt_id character varying(255),
      pdbx_auth_asym_id character varying(255),
      pdbx_auth_atom_name character varying(255),
      pdbx_auth_comp_id character varying(255),
      pdbx_auth_seq_id character varying(255),
      pdbx_formal_charge integer,
      pdbx_ncs_dom_id character varying(255),
      pdbx_struct_group_id character varying(255),
      pdbx_tls_group_id character varying(255),
      refinement_flags character varying(255),
      refinement_flags_adp character varying(255),
      refinement_flags_occupancy character varying(255),
      refinement_flags_posn character varying(255),
      restraints character varying(255),
      symmetry_multiplicity integer,
      thermal_displace_type character varying(255),
      type_symbol character varying(255)
);
```

MANY MORE TABLES NOT SHOWN (but available upon request).

The term "use in commerce" means the bona fide use of a mark in the ordinary course of trade, and not made merely to reserve a right in a mark. For purposes of this Act, a mark shall be deemed to be in use in commerce--
(1) on goods when—
(A) it is placed in any manner on the goods or their containers or the displays associated therewith or on the tags or labels affixed thereto, or if the nature of the goods makes such placement impracticable, then on documents associated with the goods or their sale, and
(B) the goods are sold or transported in commerce, and
(2) on services when it is used or displayed in the sale or advertising of services and the services are rendered in commerce, or the services are rendered in more than one State or in the United States and a foreign country and the person rendering the services is engaged in commerce in connection with the services.

Here the schema affixes the tag or label "virion" to the SQL schema. In this case, the software "goods" are transported via email to another State. If Dr. Ng wished, he could have downloaded the free PostgreSQL open source database and installed the *transported* SQL schema. Given the stated intent of **VRG** is to provide both commercial and free / low cost academic access to our tools/data, this exchange of "goods" was without cost. We now have a Google Cloud Drive setup, where those granted access can download our software (*Class 09: Downloadable computer software*. For example, scripts in R, Microsoft Access, python or other tools that have database support. Typically ODBC, but our target database technologies, Microsoft SQL Server and PostgreSQL each have optimized native APIs).

Excerpts from a message sent to Dr. John Westbrook. He is well-known in the protein sciences field, and in particular one of the key architects of the PDB file format and international protein data repository. I have owned the VIRION domain for a number of years. Dr. Westbrook's helpful response follows.

From: Paul Conlon [mailto:pconlon@rochester.rr.com]
Sent: Wednesday, September 07, 2011 10:32 PM
To: 'jwest@rcsb.rutgers.edu'
Subject: pdb/xml

I guess this is a hello.....and maybe at some point wondering if we can chat briefly to maybe help me sort a few things out and jump start my home efforts (that hopefully will turn into some sort of business. Just in case, I bought the rights to virion.com, so I am serious here ;-). Current thinking is to understand the schema, create my own version of the schema in a local db tool, start downloading and importing data, and the creating algorithms that assess proteins. I have ideas on how to this...maybe they've been implemented...but maybe not. I very much want to look into protein folding...or from my view...protein Unfolding. I think I have some interesting ideas on how to attack this from a non-chem perspective...but want the data as a starting point.

From: John Westbrook [mailto:jwest@rcsb.rutgers.edu]
Sent: Saturday, September 17, 2011 9:02 AM
To: Paul Conlon
Subject: Re: pdb/xml

Hi Paul,

Before getting involved in structural biology and informatics, I was very interested in imaging science and photochemistry. My undergraduate degree is in imaging science from RIT and I spent many years in the Rochester area before coming to Rutgers. My wife is also a graduate of Geneseo.

The work that we do at Rutgers for the PDB is focused on data acquisition, annotation and validation.   The data processing system that we use dictionary driven and based on a community data model the macromolecular crystallographic informationframework (mmCIF) and broadly extended by PDB for archiving other methods in experimental structural biology. The data model is described at the following sites.   The latter is an XML translation (xsd schema) of the former. mmCIF has its own syntax conventions.

http://mmcif.pdb.org/
http://pdbml.pdb.org/

If you are coming to this from a database perspective you will note that this data model does not correspond in any way to a conventional normalized database schema.   Rather, this is a specification that matches how this information is typically structured by the groups that generate and consume the data. It is very denormalized and contains multiple nomenclatures; however, all of this information is appropriately linked/related explicitly in the underlying data model so it is possible to rigorously validate the data in this denormalized form.   You will find that the mmCIF data model does conveniently map to a relational data model with the previously noted limitation.

We internally have developed C++ tools to manage the mmCIF flavor of PDB data and you will find links to these tools on the above sites.   We produce XML/PDBML data by software translation from the mmCIF data and independently check this data against the PDBML schemas that we distribute.   Our collaborators in Japan have used this XML data to populate a number native XML databases (supporting XPATH style queries); however, our focus has been mostly on relational implementations that closely match the underlying data model.   We are also working some integration with RDF/OWL using SPARQL but this is mostly in a related project, the Protein Structure Knowledgebase (sbkb.org).

Good luck with your efforts -

Regards,
John

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☐	virion.com ⋯	Active	8/3/2026	On	On	On
☐	virion.net ⋯	Active	6/23/2022	On	On	On
☐	virionresearch.com ⋯	Active	4/14/2028	On	On	On
☐	virionresearchgroup.com ⋯	Active	11/9/2023	On	On	On

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newegg

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Paul R Conlon
Virion Research
6701 County Road 12
Naples,NY 14512-9724
United States

585-374-2881

BILL TO

Paul Conlon
Virion Research
6701 County Road 12
Naples,NY 14512-9724

Visa:************9357

ORDER SUMMARY

Order Date: 5/22/2016 at 12:56PM

Order # 252336424
Invoice # 139351448

Sold and Shipped by Newegg

Product Description	Qty	Price
Shipped from NJ, USA		Tracking # 61299998790724945645
Cooler Master Hyper 212 EVO - CPU Cooler with 120mm PWM Fan Item #: N82E16835103099 Standard Return Policy	1	$29.99
	Subtotal	$29.99
	Tax	$0.00
	Super EggSaver (2-5 Bus. days)	$0.00
	Total for the Shipment(s)	**$29.99**

Order # 252336444
Invoice # 139371944

Sold and Shipped by AmaMax (USA) Since 1993

Product Description	Qty	Price
Shipped from AmaMax (USA) Since 1993		Tracking # 9400110200828034183727
Noctua NF-F12 PWM, 4-Pin Premium Quiet Fan (120mm) Item #: 9SIA9PV3H16655	1	$19.99
	Subtotal	$19.99
	Tax	$0.00
	Standard Shipping (5-7 bus. days)	$0.00
	Total for the Shipment(s)	**$19.99**

I have had steady requests to purchase the domain virion.com, which I have repeatedly refused. Here are some of the more recent requests. I have not entertained selling the domain because of my *bonafide intent to use*. Since brokers are often used to make the requests, the actual companies behind the purchase offers are typically unknown.

Search DomainSellRequests 🔍   Current Folder ▼

All Unread   By Date ▼   Newest ↓

pconlon@rochester.rr.com
RE: Re: virion.com [virion.com@domainsbyproxy.c...   10/9/2018
Replied to this previously.

donotreply@domainsbyproxy.com   ✉
FWD: Re: virion.com [virion.com@domainsbyprox...   10/9/2018
What is your price for this domain name?

pconlon@rochester.rr.com
FW: virion.com [virion.com@domainsbyproxy.co...   9/29/2018
Hi Mike, I am using this for a small biotech

pconlon@rochester.rr.com
RE: virion.com [virion.com@domainsbyproxy.com...   9/29/2018
Hi Mike, Not for sale...planned for my small

donotreply@domainsbyproxy.com   ✉
FWD: virion.com [virion.com@domainsbyproxy.co...   9/29/2018
Hello, Is this domain for sale? How much? Take

pconlon@rochester.rr.com
RE: Offer to buy VIRION.COM   9/18/2018
You bet Narendra! And thanks for the kind words

Narendra G   ✉
Re: Offer to buy VIRION.COM   9/18/2018
Hello Paul, Thanks for your email. I appreciate it.

pconlon@rochester.rr.com
RE: Offer to buy VIRION.COM   9/18/2018
Hi Narendra, Thanks for your contact and

Narendra G   ✉
Offer to buy VIRION.COM   9/18/2018
Good Afternoon Paul,

TierraNet Customer Care
Domain for sale inquiry (virion.com)   1/2/2018
Dear valued customer, Someone may be

Paul Conlon
RE: Virion.com   12/18/2017
Hi Charles, No plans to sell – in fact I just

Charles Parker   ✉
Virion.com   12/18/2017
Hope you're doing well. Can you give me a price

TierraNet Customer Care   ✉
Domain for sale inquiry (virion.com)   11/28/2017
Dear valued customer, Someone may be

TierraNet Customer Care
Domain for sale inquiry (virion.com)   9/18/2017
Dear valued customer, Someone may be

Paul Conlon
RE: Virion.com   6/2/2017
Hi Scott, I have my own plans for it, hopefully

📩 Reply 📩 Reply All 📩 Forward

Mon 12/18/2017 6:14 PM

Paul Conlon <pconlon@rochester.rr.com>

RE: Virion.com

To   ☐ 'Charles Parker'   ⌃

Hi Charles,

No plans to sell – in fact I just renewed/extended it and plan to start developing it this coming year. Thanks for your interest.

Best regards,
Paul

From: Charles Parker [mailto:cparker0021@gmail.com]
Sent: Monday, December 18, 2017 8:48 AM
To: pconlon@rochester.rr.com
Subject: Virion.com

Hope you're doing well.
Can you give me a price for this domain?

Thanks
C Parker