



# Interfacing PV in Galaxy

RPBS, U Paris Diderot, 28-Jun-2017

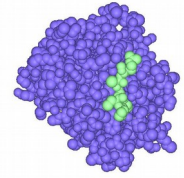
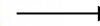
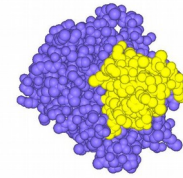
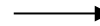
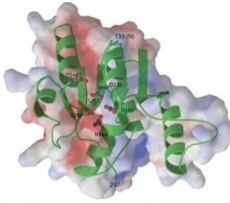
**Antoine Chemardin (engineer), Inria Nancy / LORIA**

**Dave Ritchie (coordinator), Inria Nancy / LORIA**

## 3D Visualisation

```

-----MQS
TARSRQRLVPRGGSTKRSLESLREEDREGSD---
DHKEI A I L V D V Q V V Y T C R E A Y R S N E D Y N Q E - W Y V A T
---L P V V I D G S N V A M S H G N K E V F S G R G I L L A W N W E L
LEK--E V--V---SAK A M A I A S N D K R Q H H I E R E V
R R H T D I T V F V S W R K E Q R R R V I T O H I E R E - L E K K
G F E V M L K P Y I Q R D S A K G D W V G I T L D -- A I E I A P D V
K L L V E T - R S R - V G G K R V V C Y D --- D R F E M K L A R E S
R R V I L V S C G D F S L L V - E K I Q R Y N K - V T V Y G - V --
D G V M - V S N D - T E R D L G G E R Q E W R F I E E L L M S F M N D
R R E T S Q T - L
K F M P R D D L L
  
```



- 3D visualisation is very important for molecular modeling
- Many high quality desktop tools already exist – e.g. VMD, PyMol, ...
- These all use OpenGL to exploit graphics hardware (nVidia, Radeon, Intel, ...)

## 3D Web Interfaces ?

- Until recently, the only software available was Jmol / JSmol (non-OpenGL)
  - Web interfaces for 3D graphics were very low quality & slow
- New HTML-5 offers access to hardware through “WebGL” (PV, NGL, webmol, ...)

## PV + Galaxy

- We chose PV as the “best” WebGL-based viewer for 3D protein structures
- We chose Galaxy as the “de facto standard” bioinformatics work-bench



# PV – JavaScript Protein Viewer

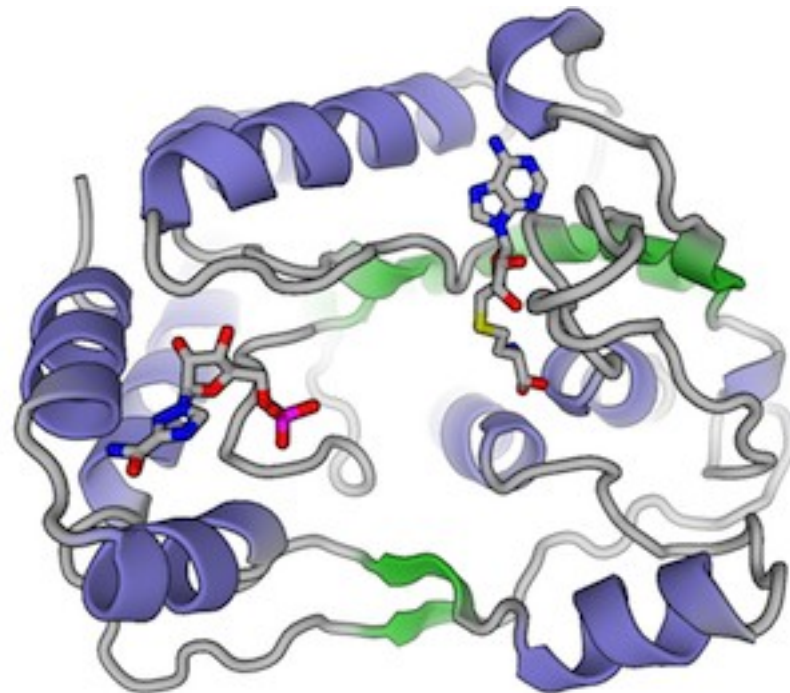
<https://biasmv.github.io/pv/>

## About PV

- Developed by Marco Biasini (SwissProt)
- Open source JavaScript + WebGL
- Used in PDB and SwissProt web sites

## Features

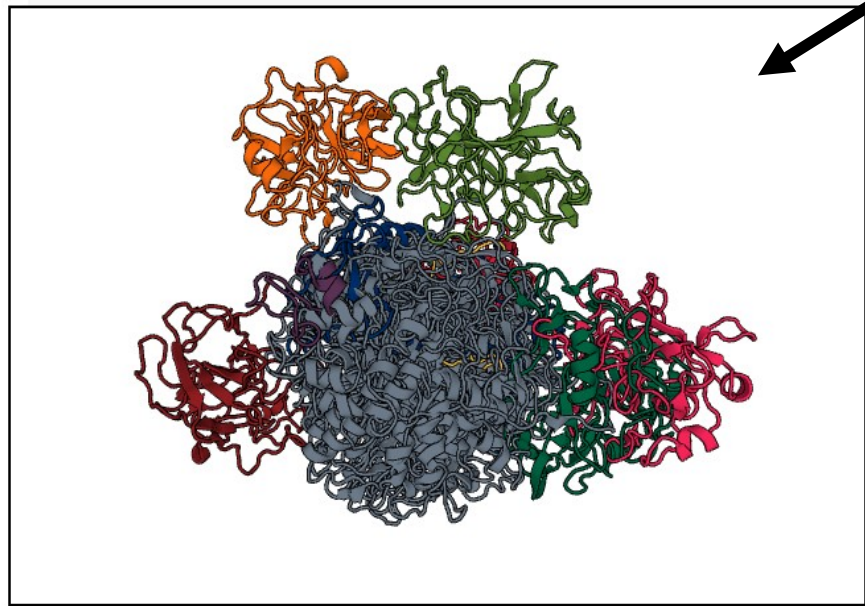
- Good JavaScript API
- Good documentation and example scripts
- Handles multiple proteins simultaneously
- Supports many ways to render proteins:
  - Ribbon cartoons
  - Ball-and-stick
  - ... etc.



# PV in HTML+JS Web Page (KBdock)

<https://kbdock2.loria.fr> (no login needed)

Superposition for Serpin (PF00079)



Interactions

- All
- PF00079\_3h5c\_A\_58\_420\_PF00089\_B\_146\_354
- PF00079\_1f0c\_A\_111\_352\_PF00079\_B\_361\_391
- PF00079\_4dy7\_F\_15\_379\_PF00089\_E\_16\_238
- PF00079\_1jmo\_A\_111\_477\_PF00089\_H\_16\_238

Sites

3  
4  
5  
6  
7











Background color

White  
 Black

WebGL window

Javascript selection tools

### Legend

-  PF00079\_2x0b\_F\_78\_448\_PF00026\_E\_14\_331\_sse.pdb
  -  PF00079\_1f0c\_B\_361\_391\_PF00079\_A\_111\_352\_sse.pdb
  -  PF00079\_2d26\_A\_31\_351\_PF00089\_C\_21\_238\_sse.pdb
  -  PF00079\_1oc0\_A\_13\_379\_PF01033\_B\_3\_39\_sse.pdb
  -  PF00079\_1k9o\_I\_22\_386\_PF00089\_E\_16\_238\_sse.pdb
  -  PF00079\_1jmo\_A\_111\_477\_PF00089\_H\_16\_238\_sse.pdb
  -  PF00079\_4dy7\_F\_15\_379\_PF00089\_E\_16\_238\_sse.pdb
  -  PF00079\_1f0c\_A\_111\_352\_PF00079\_B\_361\_391\_sse.pdb
  -  PF00079\_3h5c\_A\_58\_420\_PF00089\_B\_146\_354\_sse.pdb
  -  Query
- Javascript labels



# PV Programming – HTML Side

In the HTML code “div”s identify the JS parts:

```
<html>
<body>
<div class="row">
  <div class="col-md-8" id="viewerwrap">
    <div id="viewer"></div>
  </div>
  <div class="col-md-4"> <select id="interactions">
    <option value="structure-1.pdb" </option>
    <option value="structure-2.pdb" </option>
    ...
  </select>
</div>
</div>
...
</body>
<script src="../js/pv-bio.min.js"></script>
<script src="../js/pvviewer.js"></script>
<script> $(document).ready(function() {}) </script>
</html>
```



# PV Programming – JavaScript side

In the JavaScript code (our file ../js/pvviewer.js):

```
// define viewer rendering options
```

```
var options = {width: 'auto', height: 435, antialias: true, quality: 'medium',  
              fog: 'false', forceManualAntialiasing: false, background: 'white' };
```

```
// insert PV in the div named 'viewer'
```

```
var viewer = pv.Viewer(document.getElementById('viewer'), options);
```

```
$(function() { // launch the viewer
```

```
    document.getElementById('viewer').addEventListener('mousemove',  
                                                       function(event) {
```

```
        // more stuff here for handling mouse events ...
```

```
    });
```

```
    pv.io.fetchPdb(prot, function(structure) {
```

```
        // more stuff here for loading and processing a PDB file...
```

```
    });
```

```
});
```







# PV Programming in Galaxy

In Galaxy tool definition, set output format = "html"  
Example: /galaxy/tools/kpax/kpax.xml

```
<tool id="kpax" name="Kpax" version="1">
  <input>
    // define command input parameters and options here (not shown)
  </input>
  <outputs>
    <data format="zip" name="output_zip"
          label="{query_structure.name}_{tool.name}_zip">
    </data>
    <data format="html" name="html_file" label="Kpax Visu">
    </data>
  </outputs>
  <command>
    // run script to execute Kpax (also generates html results page)
    /kpax/kpaxwrapper.sh $html_file -nosubdirs
                          -sort="$sort_by" -top="$advanced.top"
                          -show="$advanced.show" ...
  </command>
</tool>
```





# PV – On-Line Resources

## PV Base Distribution

<https://biasmv.github.io/pv>

## PV Documentaion & Examples

<http://pv.readthedocs.io>

## PV + Galaxy from Inria Nancy

<https://gitlab.loria.fr/capsid/> (request password)

## Inria/LORIA Galaxy instance with PV + Kpax + Hex

<https://galaxy.loria.fr/> (login required)



# PV – Conclusions

## Advantages

- Relatively easy to program in JavaScript
- Good documentation & examples
- Can load arbitrary number of protein structures
- Easy to customise (picking, coloring, mouse interaction, ...)
- Original developer responds to questions + bug reports

## Disadvantages / Limitations

- Requires JavaScript (which is no longer acceptable for NAR web server)
- Has many advanced features – colour by residue, measure distances, ...
- The API seems to encourage nasty (recursive-style) function invocation
- Needs secondary structure definitions in PDB files
- Does not yet support orthographic viewport...



Thank You !

Questions ?