GenApp: Extensible Tool for Rapid Generation of Web and Native GUI Applications

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## Outline

- Background on GenApp
- Dynamic User interface from "static" definition files
- Alexey's perspective

## **CCP-SAS**

- SASSIE http://www.smallangles.net/sassie
  - Joseph Curtis et al.



National Institute of Standards and Technology = Technology Administration, U.S. Department of Commerce

- PYTHON
- includes wrapped binary executables
- SCT/SCTPL/HYDRO http://www.ucl.ac.uk/smb/perkins
  - Steve Perkins et al.

# **DCL**

**Neutron Resear** 

- Structural Immunology Group at University College London
- FORTRAN
- US-SOMO http://somo.uthscsa.edu
- \*
- Emre Brookes et al.
- C++/Qt



- includes wrapped binary executables
- attract others ...

# Bio-SAS – a variety of time scales and computational requirements



## Considerations

- **Ease of deployment** in an ever-evolving software environment landscape
- Legacy and frequently specific lab developed codes
- Labs frequently can not afford a dedicated software team nor the cost in time and funding

"Dark code"

An Open Extensible Multi-Target Application Generation Tool for Simple Rapid Deployment of Multi-Scale Scientific Codes

Brookes, E. H. XSEDE 14 Atlanta



## Definition file driven generation



#### Insure preservation in two ways



## GenApp from the "Researcher" perspective

- Given an existing executable:
  - Create a definition file describing inputs and outputs
  - Wrap or modify that executable to accept inputs and outputs as defined
  - Run the GenApp "compiler"
  - $\bullet \longrightarrow$

#### → A fully functional Science Gateway

- Users, user management and statistics
- Job management, reattach
- "Cloud" file system
- Optional messaging for "live" updates
- Caching
- Multiple execution models
  - Iocal to remote HPC and cloud
    - Airavata integration
    - OpenStack
- Can also simultaneously create "GUI" applications over the same modules
  - e.g. QT, JAVA
- Extensible!
  - features added on an as-needed basis

#### Some GenApp generated Gateways

#### In production:

SASSIE-web (J.E. Curtis) SCT (S. Perkins) https://sasssie-web.chem.utk.edu/sassie2 40 modules 350+ users, 10,000+ jobs in 2016, 40+ papers

BayesApp (S. Hansen) Denfert (J. Perez) Vortex Shedding (A. Perlstein)

#### Alpha

NAMDrunner (A. Savelyev)

http://genapp.rocks/bayesapp http://genapp.rocks/denfert http://genapp.rocks/vortexshedding

http://genapp.rocks/namdrunner







## Dynamic UI's from static definition files

```
"moduleid" : "energy"
,"label" : "Energy"
,"help" : "help for Energy"
,"executable" : "energy"
,"fields"
                       : "input"
         "role"
         ,"id" : "m"
,"label" : "mass [kg]"
,"type" : "float"
         ,"required" : "true"
         ,"help" : "Enter the mass in kilograms"
                      : "input"
         "role"
         "role" : "input"
,"id" : "c"
,"label" : "Speed of light [m/s]"
,"type" : "float"
,"default" : 299792458
         ,"required" : "true"
         ,"help"
                         : "Enter the speed of light in meters/second"
    , {
         "role" : "output"
         ,"id" : "e"
         ,"label" : "Energy [J]"
         ,"type"
                         : "text"
```

## Dynamic UI's from static definition files

• How to best define interactivity in a single definition file that can be handled within the UI?

## Dynamic UI's – repeaters & repeats





## Dynamic UI's – Calculated fields



- Can be chained
- Can be under repeaters context is managed

#### Resources

#### http://genapp.rocks & esp. http://genapp.rocks/wiki

- Primary host at University of Tennessee Knoxville
  - "Entropy" server 128 core, 256 GB ram, 8 Tesla K20m GPUs, Rocks OS
  - Running HTML5/PHP
- Indiana University Quarry nodes
  - Trac wiki with integrated subversion repository
  - Testing node
- XSEDE Jetstream
  - XSEDE ECSS vortexshedding gateway
  - SASSIE-web instance
  - NAMDrunner
- AWS
- XSEDE TG-MCB140255 Computational support for small angle scattering for advanced analyses of structural data in chemical biology and soft condensed matter
- ORNL Titan, UK SCARF (pending)

#### **Resources – Personnel**

- Alexey Savelyev
  - Target language developer
  - Application developer
  - Module wrapper
- Emre Brookes
  - Primary developer
- External Application/Module developers
  - Joseph Curtis, PI and personnel
    - SASSIE
  - David Wright
    - SCT
  - Arne Perlstein, PI's assigned personnel (currently Josef Sabuda)
    - Vortexshedding

#### Future

- Ongoing
  - More application & module wrapping
    - Training others to wrap (and making it as easy as possible)
    - We could wrap a lot given sufficient resources
  - Easy install of applications for setup of web-servers and standalone
- Near future
  - Instance generator / VM's and/or simple JSON
  - Identity management
  - Module portal
  - API access
  - Containerization
- Further out
  - Apache membership
  - Automatic regression testing

#### **GenApp Based Science Gateways**

- US-SOMO https://somo.chem.utk.edu/somo
- WillItFit https://somo.chem.utk.edu/willitfit
- QuaFit https://somo.chem.utk.edu/quafit
- Mulch https://somo.chem.utk.edu/mulch
- ParamMD https://somo.chem.utk.edu/parammd
- NAMDrun http://js-170-47.jetstream-cloud.org/namdrunner

(Nov 2015 - present)

- SASSIE https://somo.chem.utk.edu/sassie2
- Denfert https://somo.chem.utk.edu/denfert
- BayesApp https://somo.chem.utk.edu/bayesapp
- Vortexshedding http://js-172-198.jetstream-cloud.org/vortexshedding

#### Encountering GenApp (... as a researcher ...)

Underlying codes written in different languages, can be GUI or command line applications:

- C++, Python, Fortran etc.
- C++ wrapped in Python (WillItFit); C++ bundled with Qt (US-SOMO)

"Divorce" GUI from the computational component:

Create a "command-line" analogue: [./program < {arguments}]</li>

#### Wrap a command-line application:

- Application arguments and output are JSON strings of key-value pairs, {"binsize\_id": 0.2, "filename\_id": "trajectory.dcd" etc.}
- These key-value pair are described in the application (module) definition file
- Different languages can be used to parse JSON input and transfer it to the underlying application (Python, Perl, C++)

"GenApp", i.e. compile application and generate a web site.

#### Encountering GenApp (... as a researcher ...)

JSON parsers – different languages:

```
#!/usr/bin/perl
#!/usr/bin/python
                                                                                                          PERL
                                         PYTHON
import json
                                                            use JSON:
from StringIO import StringIO
                                                            if ( !@ARGV )
if (len(sys.argv) < 1):</pre>
    print "\{\"error\":\"called with no arguments\"\}\n"
                                                               print "\{\"error\":\"called with no arguments\"\}\n";
    exit()
                                                                exit:
json variables = " "
                                                            $ison = shift:
argv_io_string = StringIO(sys.argv[1])
                                                            $json_variables = decode_json( $json );
json_variables = json.load(argv_io_string)
                                                            $mass = $$json_variables{ "mass" };
            = json variables['mass']
mass
                                                            $speed_light = $$json_variables{ "speed_of_light" };
speed_light = json_variables['speed_of_light']
                                                            #.... Energy Calculation .... #
#.... Energy Calculation .... #
                                                            $output_res = {};
output_res = {}
                                                            $$output_res{ "energy" } = energy;
output_res[ 'energy' ] = energy
                                                            print encode_json( $output_res ). "\n" ;
print json.dumps( output_res )
                                   Mass [kg]
                                                         200
                                   Speed of light [m/s] 299792458
                                   Submit Reset to default values
```

Energy [] 17975103574736000000

#### Input menu for 'QuaFit' module



Output of the 'QuaFit' module



#### **QuaFit - Beta:**

- Underlying code: Fortran
- Wrapped in PERL

(~2000 lines)

#### **Encountering GenApp: Extending Horizon**

#### Cool stuff:

- Modifying fragments of code
- Adding new /Extending types
- Conditional code generation
- Browser compatibility
- Admin utilities

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#### Web Development:

HTML5 CSS JavaScript (jQuery) PHP MongoDB



#### Advanced "GenApping": WillItFit (1)

• Uploading parameter file, lrfile.input (numerical values, whitespace\_separated etc.)

Elliptic Cylinder			-			
LOAD FILE: Parameter 1:	Load parameters from	n file Fit:: 🔿 Min:	. 0.90	Value: 1.00	Max: 1.10	
Parameter 2:	ScaleN0	Fit?: O Min:	0.90	Value: 1.00	Max: 1.10	
Parameter 3:	ScaleX	Fit?: 🗌 🎽	File Unload	)		
Parameter 4:	R1	Fit?:				
Parameter 5:	R2	Fit?: 🗆 : 🌌	🖉 🕛 📠 alexs	sav WORK_Emre WillIt	_Fit Data_for	_nanodisk
Parameter 6:	Height	Fit?: 🗌	Places	Name	▲ Size	Modified
Parameter 7:	BackN100	Fit?:	O Recent	Example.dat	1.5 kB	04/15/2016
Parameter 8:	BackN0	Fit?:	ft Home	Example_diff_dir.	card 1.7 kB	09/06/2016
Parameter 9:	BackX	Fit?:	Desktop	Example_mod.car	d 1.5 kB	09/06/2016
Parameter 10:	ScaleConc	<b>Fit?:</b>	Documents Downloads	Example_mod_will     Param_1.mcp     ParametersBefore	th 1.6 kB 1.8 kB e 853 bytes	09/06/2016 04/22/2016 05/04/2016
			J Music	ParamFitted.mpc	1.8 kB	05/04/2016
		1.	D Pictures	ParamFitted_chec	:k 1.8 kB	05/07/2016
		land in	🗖 Videos	ParamFitted_diff_	_n 1.8 kB	05/04/2016
			Devices ସି 206 GB V			All Files 🔻
		5 76			Cancel	Open
	Submit Reset to a	default value				

```
"role" : "input",
"id" : "param_choice_file_anis_core_shell_micelles",
"label" : "LOAD FILE: ",
"type" : "lrfile",
"setinputfromfile" : "whitespaceseparated_reverselogic",
"setinputfromfileids": "..list_of_ids..",
"repeat": "model_list_box:anis_core_shell_micelles",
"help" : "Load parameters from file"
```

Savelyev et al. Galeways 2010 @ SUSC - 3 NOVEITIDEL 2010

#### Advanced "GenApping": WillItFit (2)

• Advanced Plot2D.output options (save to file, change X-, Y-axis scales independently)



#### Advanced "GenApping": MULCh (1)

• Reading complex input files, lrfile.input (nested repeaters, non-numerical fields)

```
KinA:SDA 2:2 complex in 200mM NaCl, 50mM Tris, 150mM imidazole
                           # Number of contrast points
7
                        # D2O fraction, I(0), I(0) error, concentration (arb units.)
0.00 0.541 0.002 11.9
0.10 0.352 0.003 11.9
0.20 0.223 0.002 11.9
0.40 0.0745 0.002 26.9
0.80 0.19 0.001 11.9
0.90 0.332 0.002 11.9
1.00 0.537 0.001 11.9
                          # Number of things disolved in water
3
0.200 M NaCl
                          # Conc., M=molecule, formula, volume
                    0.0
                                 " Tris http://www.jtbaker.com/msds/englishhtml/t7111.htm
0.050 M C4H11NO3
                    0.0
                          #"
                                 " Imidazole
0.150 M C3H4N2
                          #"
                    0.0
0.95
                          # % of the exchangables that are accessible by the solvent
0.0
                          # % of the non-exch. protons in fragment 1 replaced by deuterons
                          #number of components, (next line) number of molecules, P=protein, sequence, volume
1
2 P GSHMTEELMLKSEKLSIAGQLAAGIAHEIRNPLTAIKGFLQLMKPTMEGNEHYFDIVFSELSRIELILSELLMLAKVK
EYLNLKKLIGEVSALLETQANLNGIFIRTSYEKDSIYINGDQNQLKQVFINLIKNAVESMPDGGTVDIIITEDEHSVHVTVKDE
GEGIPEKVLNRIGEPFLTTKEKGTGLGLHPEKGTAFKISFPKK 0.0
                         # % of the exchangables that are accessible by the solvent
1.00
0.85
                         # % of the non-exch. protons in fragment 2 replaced by deuterons
1
2 P GSMRKLSDELLIESYFKATEMNLNRDFIELIENEIKRRSLGHIJSVSS 0.0
```

#### Advanced "GenApping": MULCh (1)

• Reading complex input files, lrfile.input (nested repeaters, non-numerical fields)



#### Advanced "GenApping": MULCh (2)

#### Calculated fields (inter-dependent numerical fields)

CONTRAST VALUES (opt)							_		rho_1	fd20	rho_2
Vol <sub>1</sub> (Å)	65							$\Delta \rho_1 =$	155	f <sub>D2</sub> 0+	23
Vol <sub>2</sub> (Å)	40							$\Delta \rho_2 =$	435	$f_{D_2O}+$	234
CONTRAST POINTS											
Upper <i>qR<sub>g</sub></i> limit	1.3										
Number of Contrast Points:	umber of Contrast Points: 4										
	$f_{D_2O}(0-1)$	Refine Scale	Scale Value	Start Point	C	ontrast Data	Z	$1\rho_1$	$\Delta \rho_2$	$Vol_1/(Vol_1+Vol_2)$	
ſ	0.1	≤	1.0	1	Browse	No file selected.	38.5		277.5	0.6190476190	
fd20	0.2	≤	1.0	1	Browse	No file selected.	54		321	0.6190476190	
	0.3	≤	1.0	1	Browse	No file selected.	69.5		864.5	0.6190476190	
	0.4	~	1.0	1	Browse	No file selected.	85		108	0.6190476190	

{			
	"role"	:	"input",
	"id"	:	"delta_rho_1",
	"label"	:	"Delta rho",
	"type"	:	"float",
	"repeat"	:	"contrast points",
	"required"	:	"true",
	"calc"	:	"rho_1*fd2o + rho_2",
}			

#### Advanced "GenApping": ParamMD (1,2)

 Trajectory Movie generation [.mp4, .webm] video.output (new type added)



Savelyev et al. Gateways 2016 @ SDSC – 3 November 2016

Structure visualization, JSmol atomicstructure.output



- : "atomicstructure",
- "jsmoladd" : "hide HOH; spin on", : 450,

  - : 450

"width"

"height"

#### **Advanced "GenApping": Admin Utilities**

• Job History, jobs information within specified time frame (PHP, MongoDB)

≡ 🙇	NA	Lo	ogoff alexey Help on José 🖉			
	Job monitor Integ	rity check Users	User mana	agement J	ob history	
Start Date	2016-10-10					
End Date	2016-11-03					
Submit Res	et to default values					
name	email	duration (h)	running	finished	cancelled	BA
Totals		102.411	1	221	3	
alexey	alexsav.science@gmail.com	1.547	1	99	1	<u> </u>
amirayuyu	e amirayuyue@gmail.com	0	0	0	0	
cpayne	christy.payne@uky.edu	0	0	0	0	
danielma	danmart_us@yahoo.com	0	0	0	0	
emre	emre@biochem.uthscsa.edu	0.292	0	49	0	
graceb	gracebrannigan@gmail.com	0	0	0	0	
gumbart	gumbart@physics.gatech.edu	0	0	0	0	
hwang	hhwang8@gatech.edu	56.094	0	65	2	
jvermaas	joshua.vermaas@nrel.gov	44.476	0	8	0	
mocohen	mocohen@uchicago.edu	0	0	0	0	
pcardena	pacl3@gatech.edu	0	0	0	0	
genapp.roc	homas.joseph@uphs.upenn.edu	0	0	0	0	

## In closing

- GenApp produces working science gateways & local GUI apps
- Easily extensible
- Advancements are requirements driven
- So let us know your requirements!



Gateways 2016 organizing committee and the Gateways Institute

## Thanks for attending Questions: ask now or email me at emre@biochem.uthscsa.edu Acknowledgments

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