

Application Generation with GenApp

Emre H Brookes

Science Gateway Seminar

1 May 2015



Outline

- CCP-SAS
- GenApp Framework
- Future tasks

Outline

- **CCP-SAS**
- GenApp Framework
- Future tasks

- **Paul Butler (PI)**

*University of Tennessee Knoxville
NIST Center for Neutron Research*

- **Emre Brookes**

University of Texas Health Science Center San Antonio

- **Jianhan Chen**

Kansas State University

- **Joseph Curtis**

NIST Center for Neutron Research

- **Tom Irving**

Advanced Photon Source

+ other collaborators



Grant No.
SI2/CHE-1265821

An SI² cyberinfrastructure project
addressing Grand Challenges in
the Chemical Sciences

CCP-SAS Project

<http://www.ccpsas.org>

Collaborative Computational Project
for advanced analyses of structural
data in chemical biology and soft
condensed matter

Grant No.
EP/K039121/1

EPSRC

- **Stephen Perkins (PI)**

University College London

- **David Barlow**

Kings College London

- **Karen Edler**

University of Bath

- **Richard Heenan & Steve King**

ISIS Pulsed Neutron & Muon Source

- **David Scott**

Nottingham University

- **Nick Terrill**

Diamond Light Source

+ other collaborators

CCP-SAS

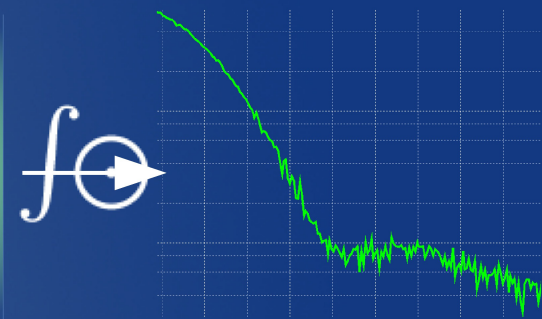
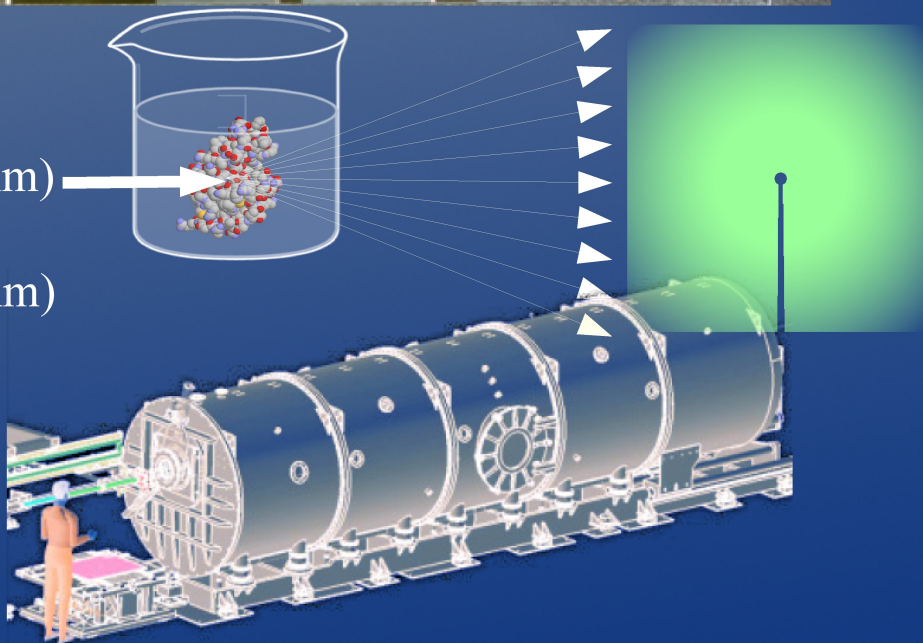
- **Collaborative Computational Project** for advanced analyses of structural data in chemical biology and soft condensed matter
 - SI2-CHE cyberinfrastructure project addressing Grand Challenges in the Chemical Sciences
- **Small Ange Scattering**



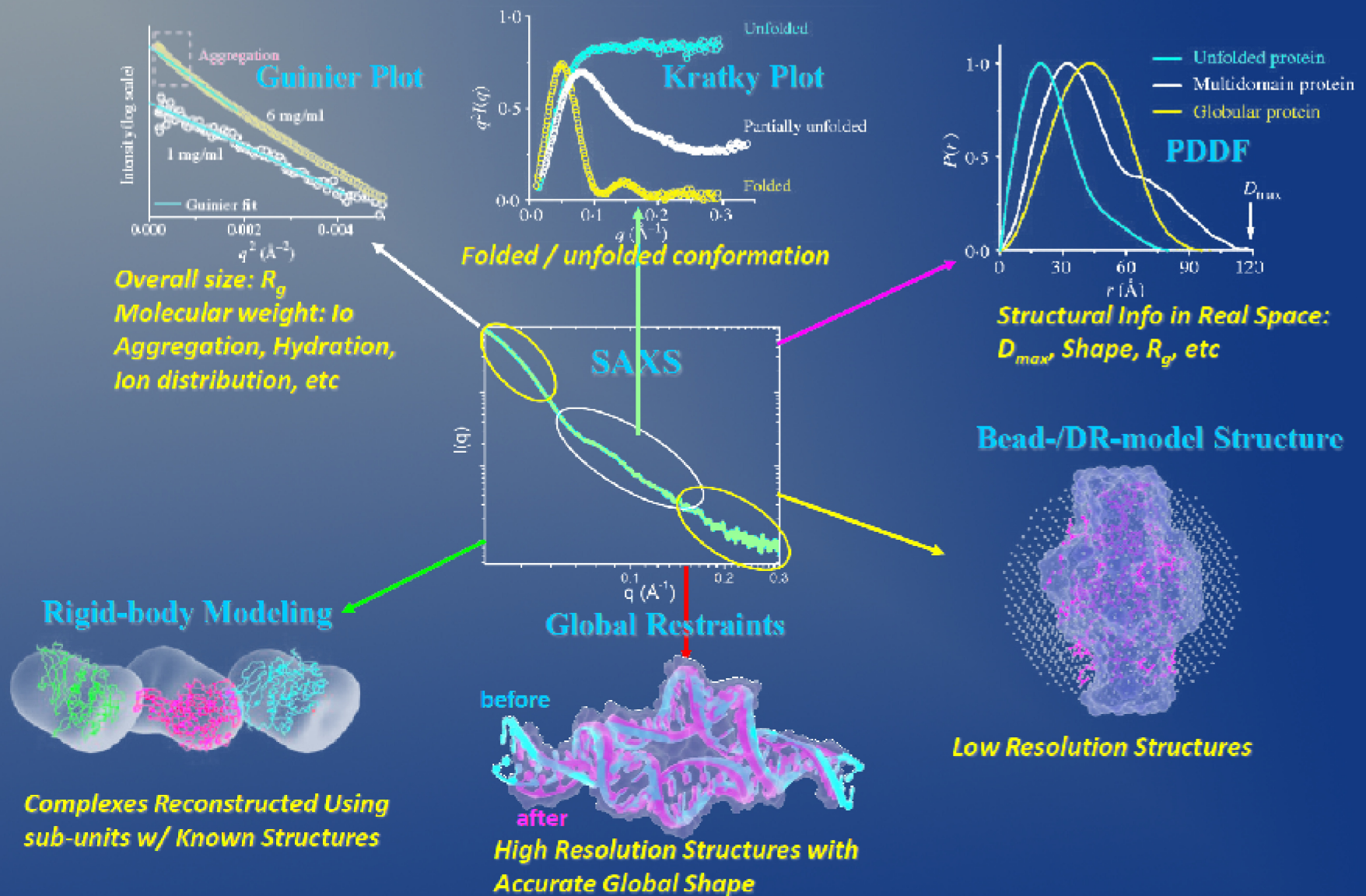
Lab X-ray ($\lambda=0.1 - 0.2$ nm)

Neutron reactor ($\lambda=0.1 - 1$ nm)

Storage Ring ($\lambda=0.03 - 0.4$ nm)



Biological solution **SAS** data processing



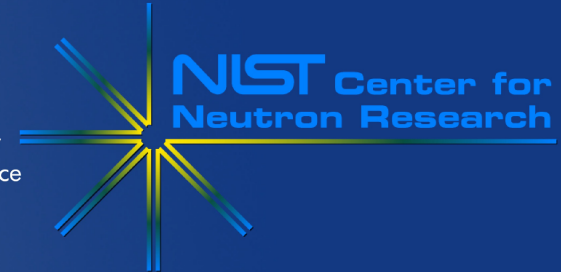
CCP-SAS

- **SASSIE** <http://www.smallangles.net/sassie>

- Joseph Curtis et al.

NIST

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.



- 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 ...

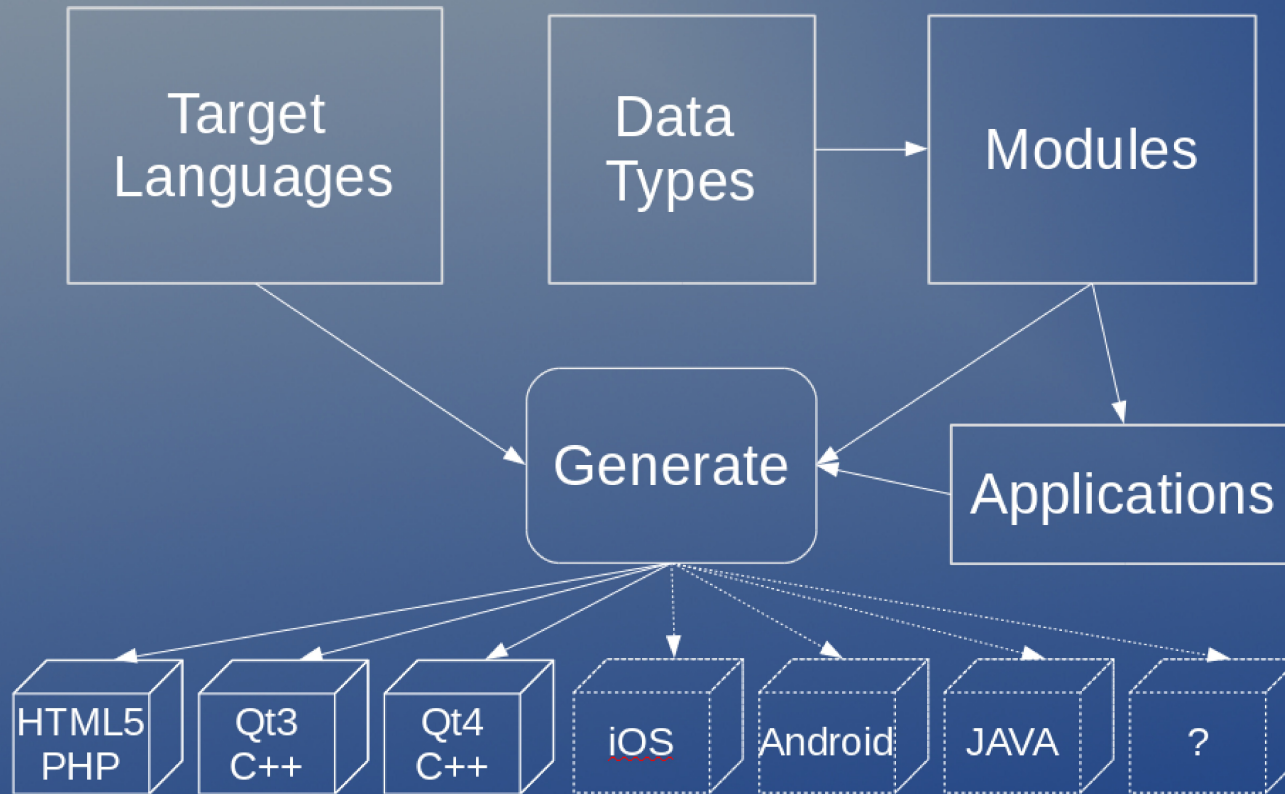


Considerations

- **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

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

Brookes, E. H. XSEDE 14 Atlanta



- JSON
- Global directives & application menu and configuration
- Module I/O definitions
- Module messaging
- Language assembly descriptions

Outline

- CCP-SAS
- **GenApp Framework**
 - **Framework user perspective**
 - **Execution model & messaging**
 - **File management**
 - **Job management**
 - **Brief demo (if time & network allows)**
- Future tasks

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extremely basic instructions to wrap an application

- from your base directory
 - edit directives.json
 - edit menu.json
 - edit modules/*.json
 - create application executable json wrappers in bin/
 - NB: executable **must** only output valid json to stdout
 - run \$ genapp.pl
 - html output should be available via web interface
 - eg
 - <http://somo.chem.utk.edu/genpptest>
 - if you get forbidden errors in the web browser, make sure everything is group readable by user apache

Credit: *Joseph Curtis – 1st User*

Directives

```
{
  "title"      : "genapptest",
  "application" : "genapptest",
  "version"    : "2.0",
  "languages"  : [ "html5", "qt3", "qt4", "qt5" ],
  "footer"     : "genapp environment",
  "footersize" : "2.5rem",

  "executable_path" :
    {
      "html5" : "/share/apps/genapp/genapptest/bin",
      "qt3"   : "/home/ehb/genapptest/bin",
      "qt4"   : "/home/ehb/genapptest/bin",
      "qt5"   : "/home/ehb/genapptest/bin",
    },

  "docroot" :
    {
      "html5" : "/share/apps/genapp",
      "qt3"   : "/tmp",
      "qt4"   : "/tmp",
      "qt5"   : "/tmp",
    },

  "helper" :
    {
      "txt" : "emacs",
      "pdb" : "rasmol"
    },

  "appconfig" : "/home/ehb/genapptest/appconfig.json"
```

```

    "text_color_rgb"      : "220,210,210",
    "error_color_rgb"     : "255,0,0",
    "background_color_rgb" : "0,0,95",
    "select_color_rgb"    : "200,128,0",
    "button_color_rgb"    : "228,255,250",
    "button_color_hex"    : "E4FFFA",
    "button_g_color_rgb"  : "128,170,150",
    "button_g_color_hex"  : "80AA06",
    "button_hover_color_rgb" : "255,255,255",
    "button_hover_color_hex" : "FFFFFF",
    "button_hover_g_color_rgb" : "228,255,250",
    "button_hover_g_color_hex" : "E4FFFA",
    "header1_color"       : "228,255,250",
    "header2_color"       : "228,255,250",
    "header3_color"       : "228,255,250",
    "header4_color"       : "228,255,250",
    "help_background_color_rgb" : "0,0,75",
    "help_text_color_rgb"  : "240,240,210"
  }
```

Application configuration

```
{
  "mail" : {
    "admin"      : "someone@someplace.net"
    , "from"      : "someotherplace.net"
    , "feedback"  : "somefeedback@someplace.net"
    , "smtp"      : {
      "host"      : "some-smtpserver.domain.net"
      , "user"     : "some-user@somewhere.net"
      , "password" : "encrypted-pw"
    }
  }
  , "hostip" : "160.36.200.43"
  , "messaging" : {
    "wsport"      : 8080
    , "zmqhostip" : "1.2.3.4"
    , "zmqport"   : 12342
    , "udphostip" : "1.2.3.4"
    , "udpport"   : 12343
  }
  , "resources" : {
    "local"       : ""
    , "compute0"  : "ssh compute-0-0"
    , "compute1"  : "ssh compute-0-1"
  }
  , "resourcedefault" : "local"
  , "submitpolicy"    : "login"
}
```


Menu Definition

```
{
  "menu" : [
    {
      "id" : "tools",
      "label" : "Tools",
      "icon" : "pngs/tools.png",
      "modules" : [
        {
          "id" : "center",
          "label" : "Center",
        },
        {
          "id" : "align",
          "label" : "Align",
        },
        {
          "id" : "data_interpolation",
          "label" : "Data Interpolation",
        }
      ]
    },
    {
      "id" : "build",
      "label" : "Build",
      "icon" : "pngs/build.png",
      "modules" : [
        {
          "id" : "build_1",
          "label" : "Build 1",
        },
        {
          "id" : "build_2",
          "label" : "Build 2",
        }
      ]
    }
  ],
}
```



Menu Definition

```
{
  "menu" : [
    {
      "id" : "tools",
      "label" : "Tools",
      "icon" : "pngs/tools.png",
      "modules" : [
        {
          "id" : "center",
          "label" : "Center",
        },
        {
          "id" : "align",
          "label" : "Align",
        },
        {
          "id" : "data_interpolation",
          "label" : "Data Interpolation",
        }
      ]
    },
    {
      "id" : "build",
      "label" : "Build",
      "icon" : "pngs/build.png",
      "modules" : [
        {
          "id" : "build_1",
          "label" : "Build 1",
        },
        {
          "id" : "build_2",
          "label" : "Build 2",
        }
      ]
    }
  ],
}
```





genapptest 2.0

Logoff emre
Help on



Center

Align

Data Interpolation

Center value 1

Minutes to run

Message results ☒

Results interval in seconds

Submit

Reset to default values

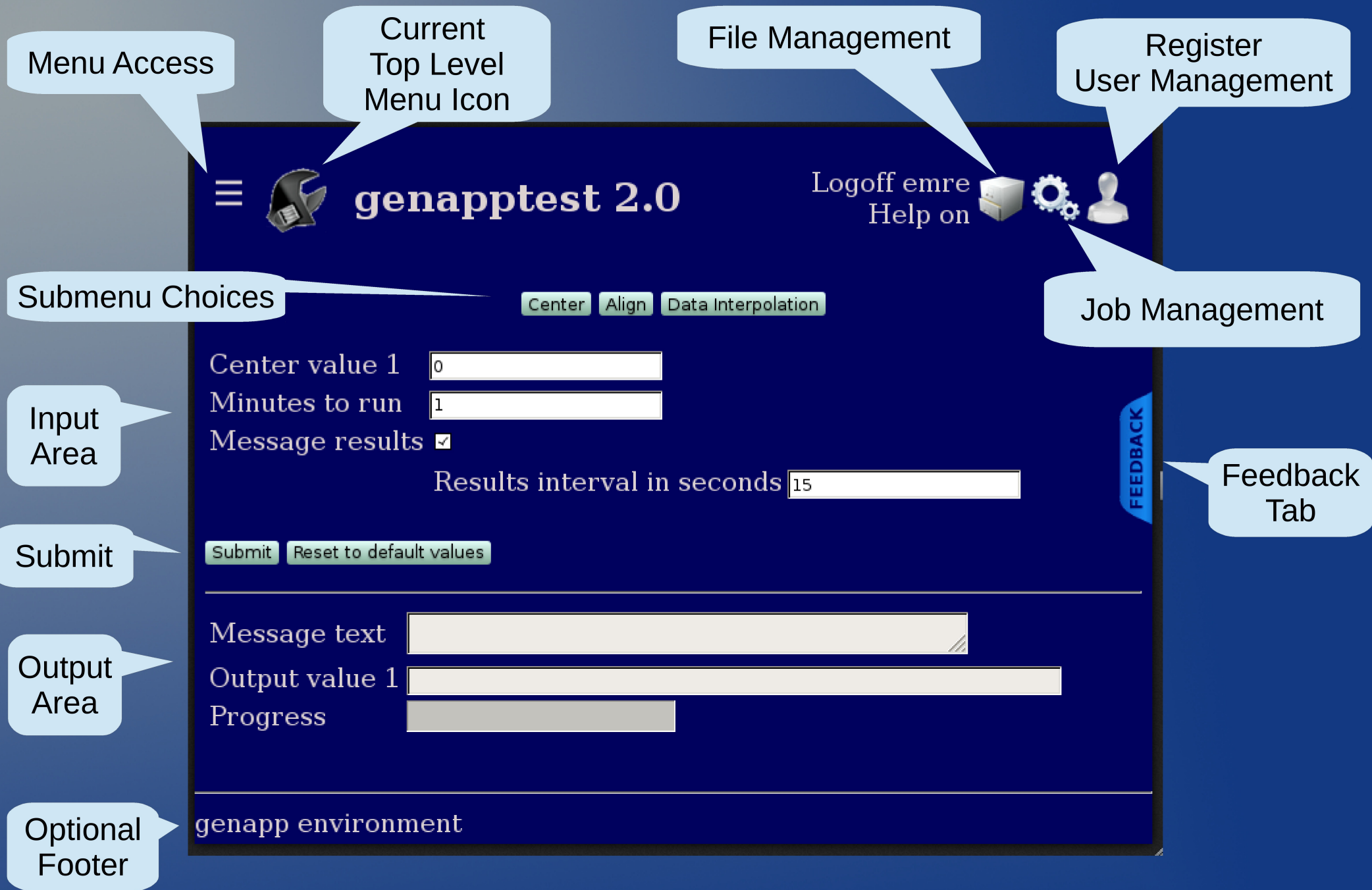
Message text

Output value 1



Progress


FEEDBACK

genapp environment



HTML5/PHP and Qt/C++ versions side-by-side

**genapptest 2.0**

Login
Help off

Center Align Data Interpolation

Start x

End x

Delta x

abs ☐

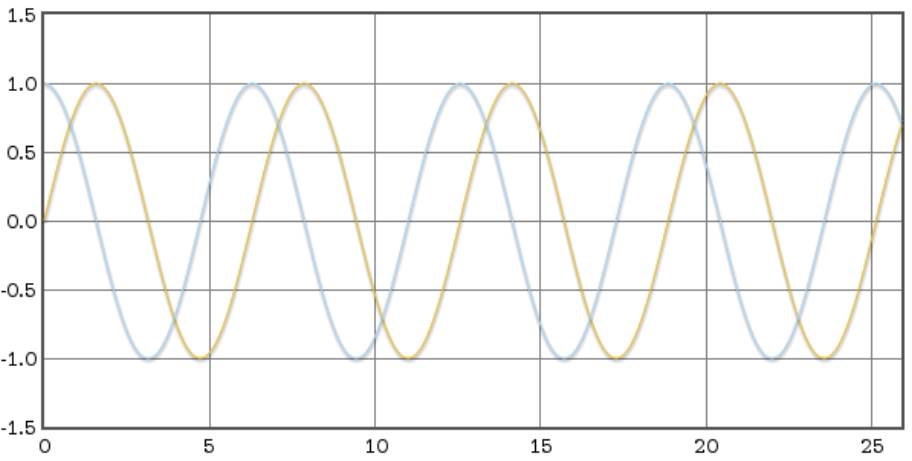
Submit Reset to default values

output integer

output float

output text



plot 2d



input json reference [logref.txt](#)

results json reference [logres.txt](#)

test pdb output [testpdb.pdb](#)

**genapptest 2.0**

Center Align Data Interpolation

Start x

End x

Delta x

abs

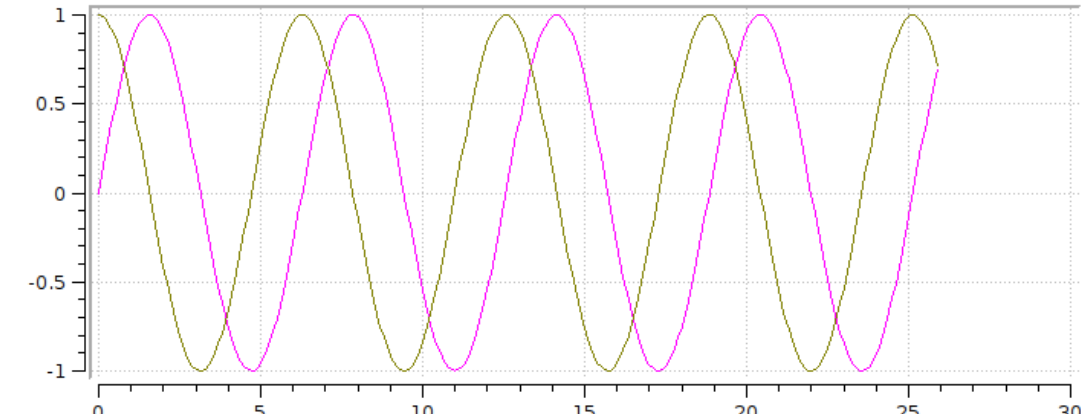
Submit Reset to default values

output integer

output float

output text

plot 2d



input json reference [/tmp/genapptest/20140323021456264/logref.txt](#)

results json reference [/tmp/genapptest/20140323021456264/logres.txt](#)

test pdb output [/tmp/genapptest/20140323021456264/testpdb.pdb](#)

2D Plot
HTML5/PHP: Flot
Qt/C++ : Qwtplot

Molecular Viewer
HTML5:JSMol
Qt/C++: Multiple options (RASMOL, Jmol, others)

genapptest 2.0

Center Align Data Interpolation

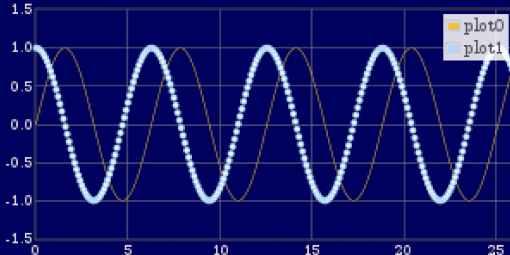
Start x: 0
End x: 26
Delta x: 0.1
abs: ☐

Submit Reset to default values

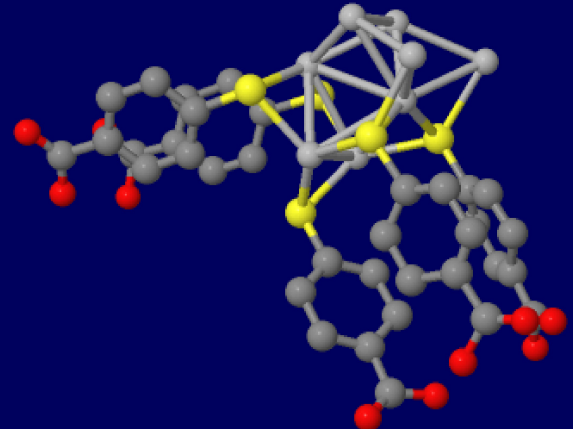
Unexpected results:
hi => data_interpolation executable
p => results/users/emre/no_project_specified

output integer:
output float:
output text:

plot 2d



input json reference: [logref.txt](#)
results json reference: [logres.txt](#)
test pdb output



Module fields

name	input support	output support	append (output-only) primarily for messaging)	default (input-only)	min (input-only)	max (input-only)	step (input-only)	required (input-only)	repeater (input-only)	help (example calculate:calculate_2, analysis:pm)	notes	genapptest example
integer	yes	yes	yes	no	yes	yes	html5-only	yes	html5-only	html5-only		tools:center repeater example interact:interact_1 step example tools:center
float	yes	yes	no	yes	yes	yes	html5-only	yes	no	html5-only		tools:center
text	yes	yes	no	yes	no	no	no	yes	no	html5-only		build:build_1
textarea	yes	yes	html5-only	yes	no	no	no	yes	no	html5-only	multiline default input not yet supported	build:build_2
checkbox	yes	yes	no	no	no	no	no	yes	html5-only	html5-only	additional 'checked' attribute	build:build_2 repeater example calculate:calculate_1
radio	yes	yes	no	no	no	no	no	yes	no	html5-only	one entry for each button name is the name of the radio button (common for all members)	build:build_2
listbox	yes	no	no	yes	no	no	no	no	html5-only	html5-only	no required attribute, but it will always have a value row spacing minor layout issue on repeater	build:build_2 repeater example calculate:calculate_2
plot2d	no	yes	no	no	no	no	no	no	no	html5-only	more info	tools:data_interpolation
atomicstructure	no	yes	no	no	no	no	no	no	no	html5-only	more info	tools:data_interpolation
file	yes	yes	no	no	no	no	no	no (always required in html5)	no	html5-only	additional multiple attribute(input-only)	simulate:simulate_1
label	html5-only	html5-only	no	yes*	no	no	no	no	no	html5-only	*can be header1,2,3,4 or blank	interact:interact_2
hidden	html5-only	no	no	yes	no	no	no	no	no	no	this is primarily to pass a value in json to the executable	analysis:pm
html	no	html5-only	no	yes	no	no	no	no	no	no	allows html output	none currently, but it's a typical field layout
progress	no	html5-only	no	no	no	yes (for output)	no	no	no	no	progress bar default ranges is 0 to 1.0, setting max to a positive value will make the range 0-max	tools:center

Module definition

```
{
  "moduleid" : "center",
  "label" : "Center",
  "executable" : "center",
  "submitpolicy" : "all",
  "fields" : [
    {
      "role" : "input",
      "id" : "input1",
      "label" : "Center value 1",
      "type" : "float",
      "default" : 0.0,
      "min" : 0.0,
      "max" : 1e50,
      "step" : 0.01,
      "required" : "true"
    },
    {
      "role" : "input",
      "id" : "runminutes",
      "label" : "Minutes to run",
      "type" : "float",
      "default" : 1,
      "min" : 0,
      "max" : 10000,
      "required" : "true"
    },
    {
      "role" : "input",
      "id" : "usemessage",
      "label" : "Message results",
      "type" : "checkbox",
      "checked" : "true",
      "repeater" : "true"
    },
    {
      "role" : "input",
      "id" : "messagesecs",
      "label" : "Results interval in seconds",
      "type" : "integer",
      "default" : 15,
      "min" : 1,
      "max" : 1000,
      "repeat" : "usemessage"
    }
  ],
}
```

```
{
  "role" : "output",
  "id" : "output2",
  "label" : "Message text",
  "type" : "textarea",
  "append" : "on",
  "cols" : 60
},
{
  "role" : "output",
  "id" : "output1",
  "label" : "Output value 1",
  "type" : "text",
  "size" : 60
},
{
  "role" : "output",
  "id" : "output3",
  "label" : "Progress",
  "type" : "progress",
  "max" : 1.0
}
]
```

Executable Input

```
{
  "input1": "0",
  "runminutes": "1",
  "usemessage": "on",
  "messagesecs": "15",
  "_logon": "emre",
  "_project": "",
  "_window": "d67fa871-46ea-4af3-d384-",
  "_uuid": "197f3ea0-a2b4-11e4-ae42-518",
  "_base_directory": "Vshare\\apps\\gena",
  "_udphost": "160.36.200.43",
  "_udpport": 37779,
  "resourcedefault": "local"
}
```

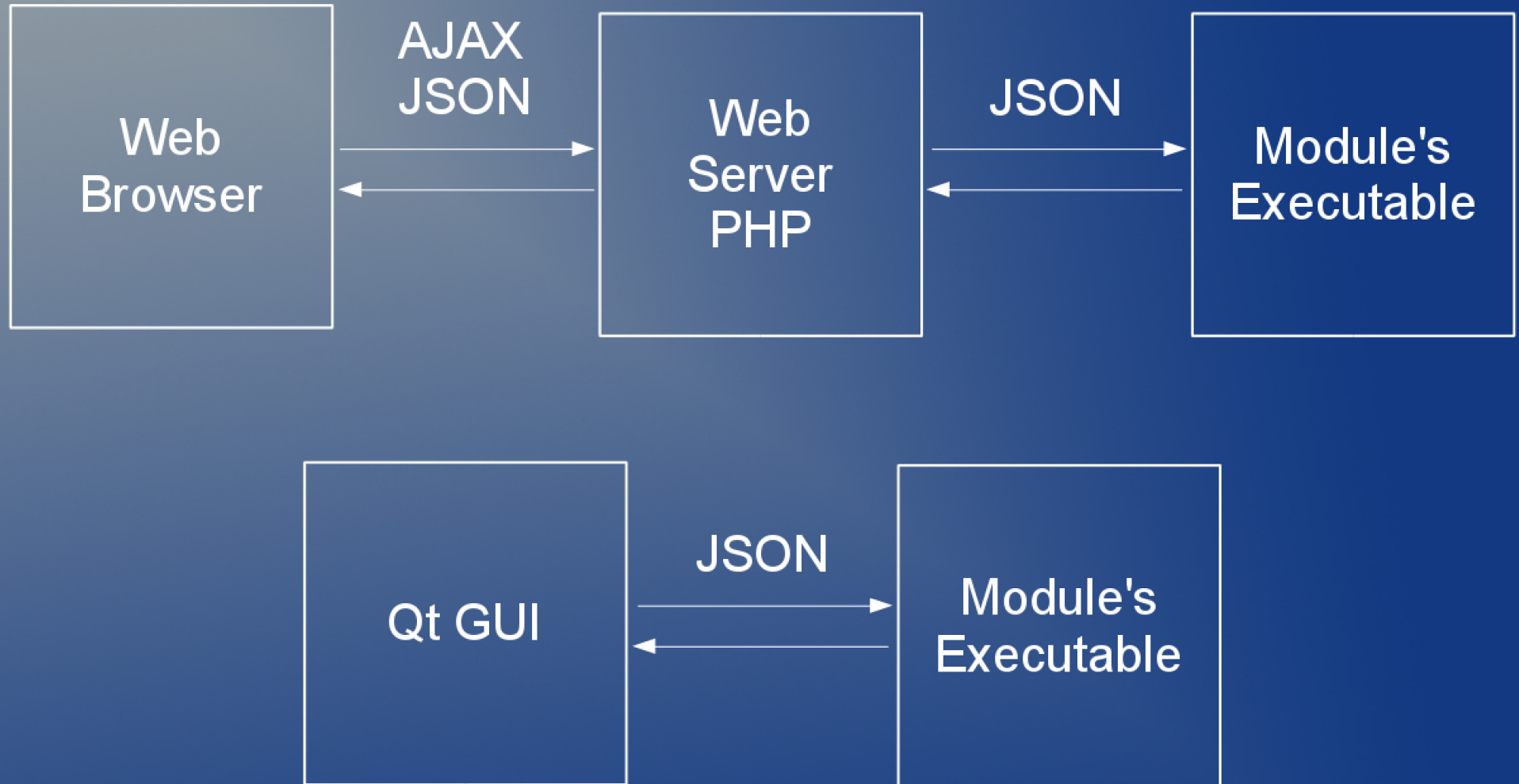
Executable Output

```
{
  "udphost": "160.36.200.43",
  "output1": "Fully completed 4 runs of sleep 15s",
  "_message": {
    "icon": "information.png",
    "text": "test message"
  },
  "output3": 1,
  "hi": "center executable",
  "udpport": 37779
}
```

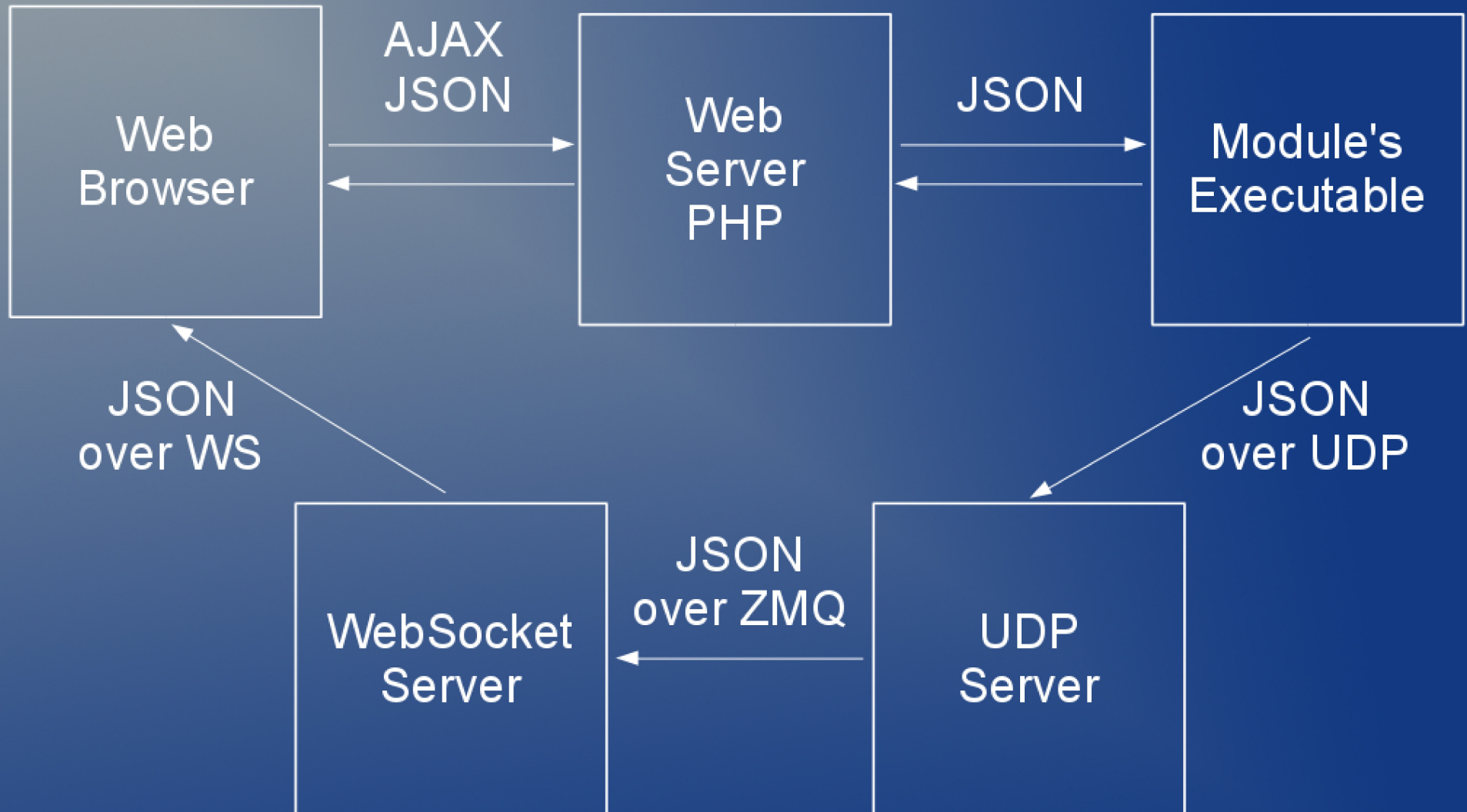
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 - **Execution model & messaging**
 - File management
 - Job management
 - Brief demo (if time & network allows)
- Future tasks

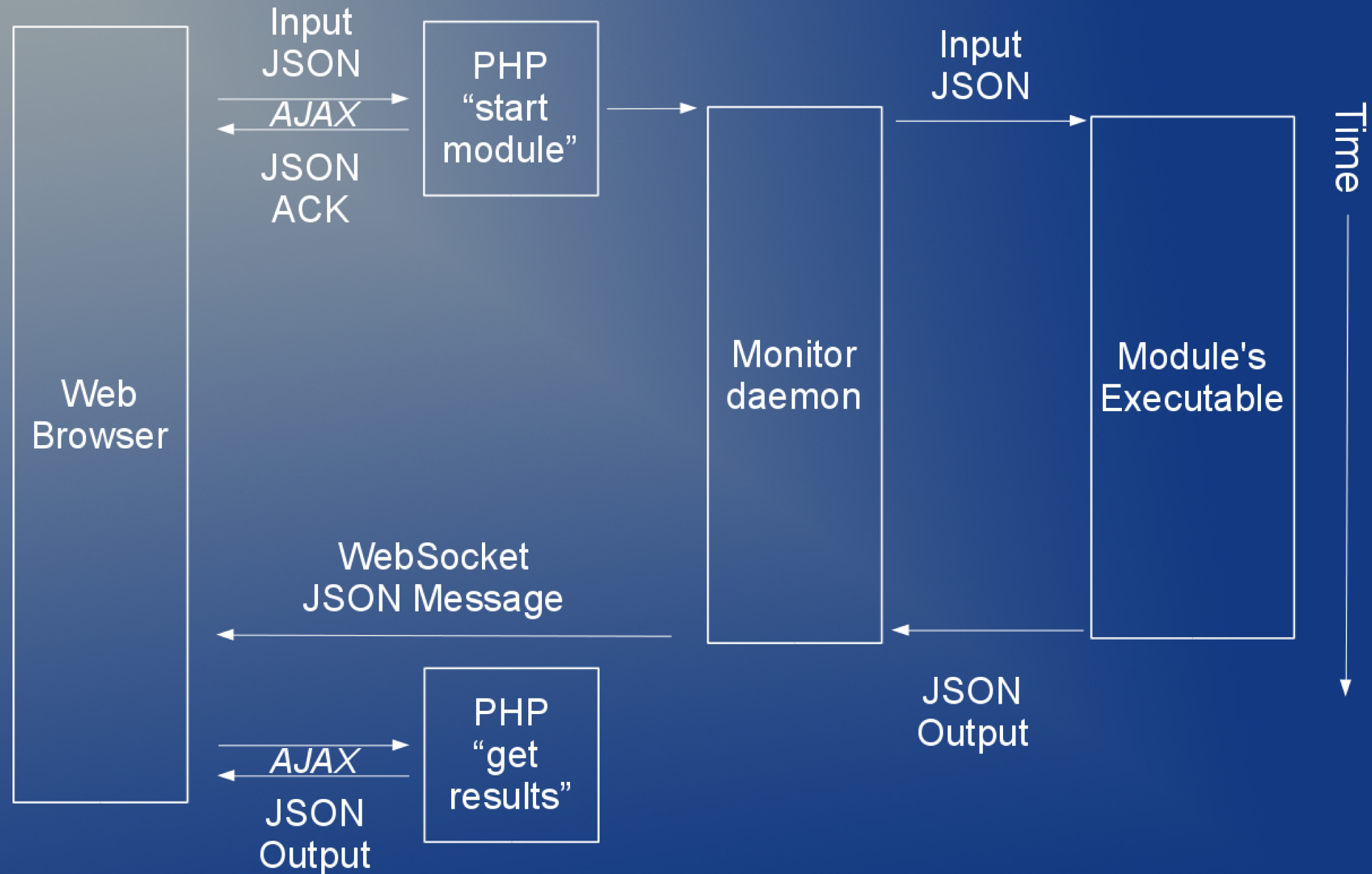
Execution model HTML5/PHP vs Qt/C++



HTML5/PHP messaging

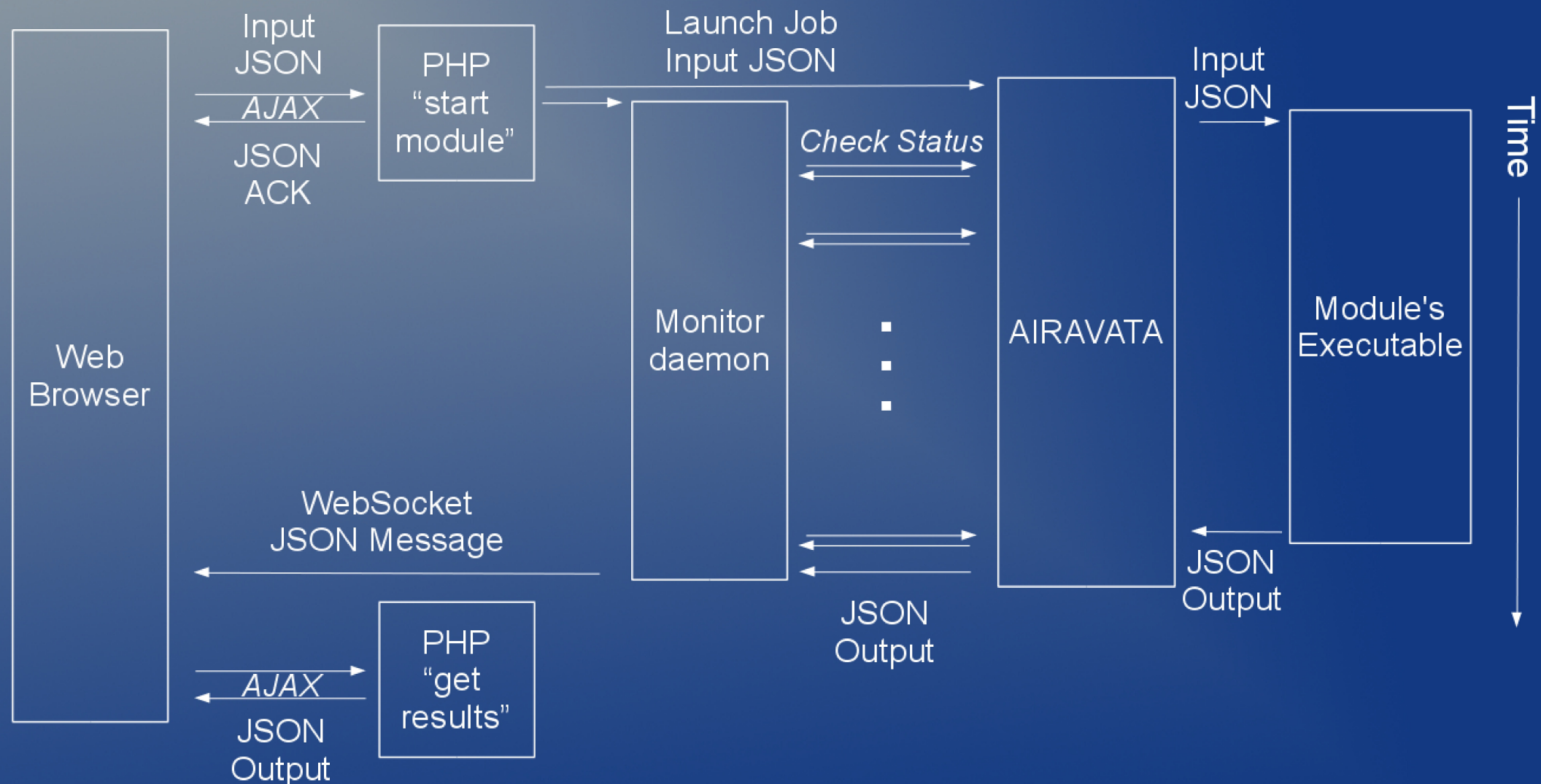


Enhanced execution model HTML5/PHP



Enhanced execution model HTML5/PHP with Apache Airavata

Nadeem Anjum
Google Summer of Code / Mentor: Suresh Marru



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File management

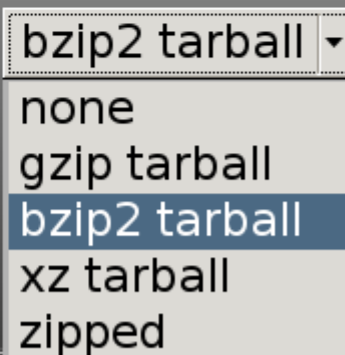
- The preferred mechanism for data input and output within the framework is formatted in JSON.
- When a module execution is submitted, a unique run directory is created for its execution.
- Files associated with the submission are placed in this directory and made available to the executing module.
- SASSIE code has cases where outputs from a previously executed module are expected to be available to a subsequent one.
- → Projects
 - Persistent directories
 - Project locking
 - File management

Files

User file tree



Compression
type



Download

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Jobs

	Module	Project	Start	End
<input type="checkbox"/>	tools/center	testproject1	2015 Jan 19 11:25:56 UTC	93.3%
<input type="checkbox"/>	tools/data_interpolation	testproject1	2015 Jan 19 11:07:42 UTC	2015 Jan 19 11:07:42 UTC

Refresh ☒ Cancel ☐ Clear Lock ☐ Remove Job ☐ Reattach ☐

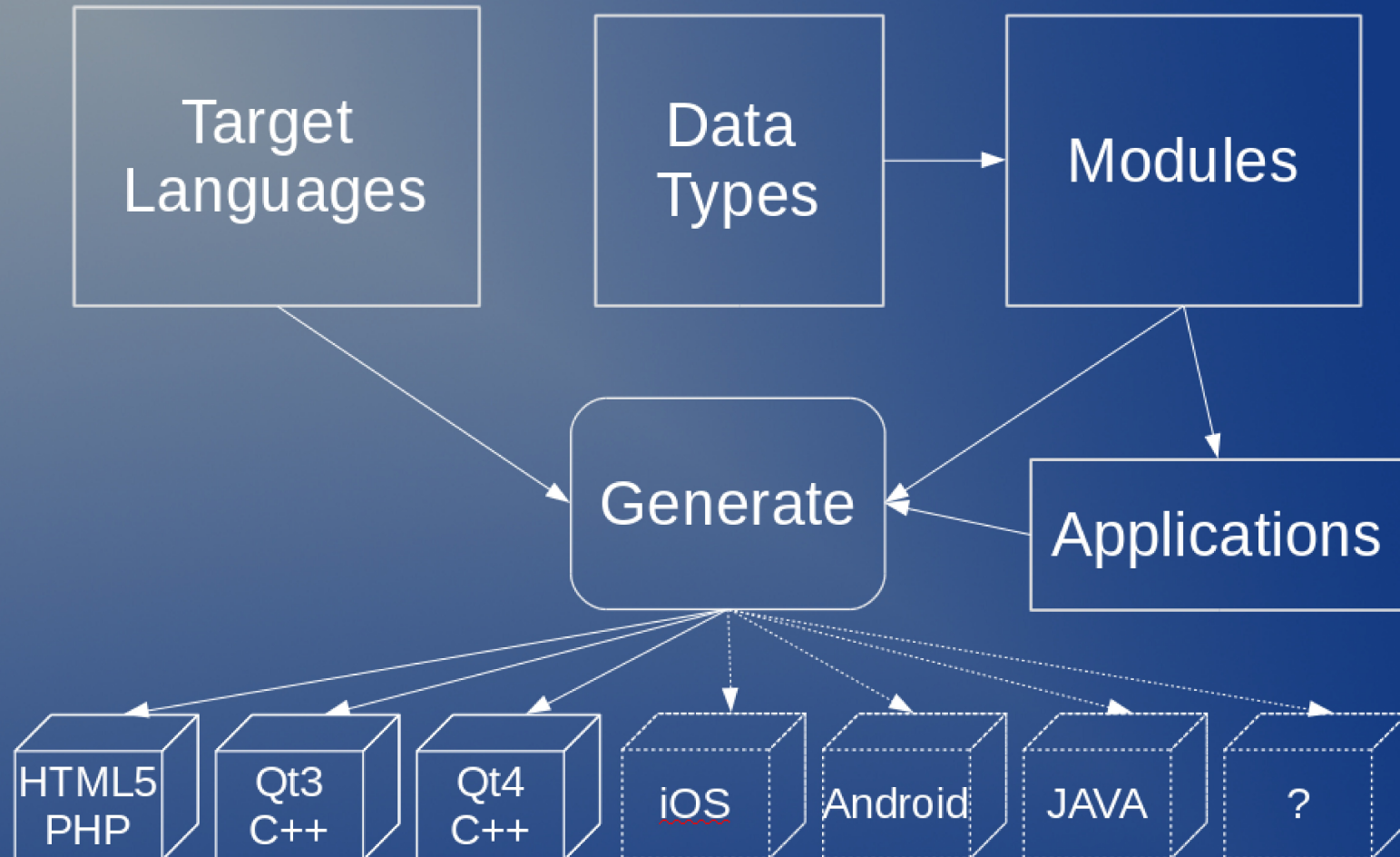
Submit

Messages

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GenApp Framework



Resources

- Current infrastructure
 - University of Tennessee Knoxville
 - “Entropy” server 128 core, 256 GB ram, 8 Tesla K20m GPUs, Rocks OS
 - Running HTML5/PHP
- Indiana University Quarry nodes
 - Testing HTML5/PHP
 - Trac wiki with integrated subversion repository
- Multiple students working at NIST
- Successful first workshop utilizing the infrastructure for SASSIE code on “entropy”
 - American Conference on Neutron Scattering 1 June 2014
- XSEDE TG-MCB140255 *Computational support for small angle scattering for advanced analyses of structural data in chemical biology and soft condensed matter*
- ORNL Titan 10% (pending)

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Future tasks

- New target languages (GSoC)
 - JAVA
 - Qt5 → iOS & Android
- Wrapping US-SOMO code into the framework (post-Doc)
- Integration with latest Airavata (GsoC)
- Advances in job management
- Apache Incubator

Thanks for listening

*Questions: ask now or
email me at emre@biochem.uthscsa.edu*

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- To E. Brookes
 - NIH NIGMS K25GM090154 / PI
 - NSF CHE-1265817 / PI
- NSF XSEDE TG-MCB140255
- UTHSCSA BCF
- To N. Anjum
 - Google Summer of Code

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