afspm: A Manufacturer-Agnostic Automation Framework for SPM

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Outline

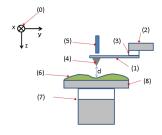
1 Justification

2 Introduction to afspm

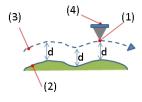
3 Design Particulars

SPM Basics

- An atomically-sharp tip is scanned above a surface measuring properties.
 - Allows spatial imaging, spectroscopic analysis, sample manipulation.
- Usable on various surfaces, only require relatively flat sample ($\sim 5 \mu m$).



Typical AFM Configuration, Tom Toyosaki, Wikimedia Commons.



Schematics of AFM topographic image forming, Tom Toyosaki, Wikimedia Commons.

Challenges and Automation

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Challenges for Wider Adoption

- Preparing, running, and analyzing requires significant domain knowledge.
- 2 Running an experiment requires constant user attention.
- **3** Statistical understanding is limited by the researcher's decisions.

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Automation Prior Art

- Conditioning of the tip for proper surface characterization.
- Structure classification, for where to scan next.
- Bayesian/Active Learning for statistical decision making.

A Remaining Limitation

Many SPM systems allow custom scripts to run an experiment. But:

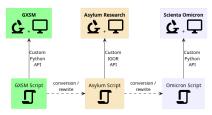
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Justification

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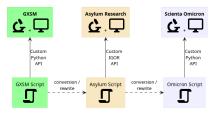
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Code reuse is rare.

Design Particulars

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Concerned with the choices a researcher would perform during an experiment.

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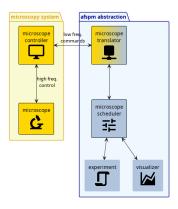
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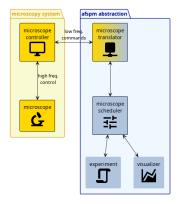
Design Characteristics

- Standalone components that each 'do one thing and do it well' (nodes).
- They communicate over 'pipes' via generic schemas.
- It is easy to **split up** components among **different** computing **devices**.

Principal Components



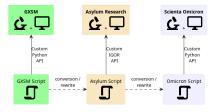
Principal Components



Any experiment must contain:

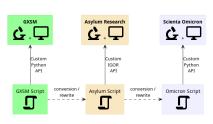
- Microscope Translator: translates between afspm-generic and microscope-specific.
- Microscope Scheduler: mediates control between components and translator and caches data.

Scripting with / without afspm

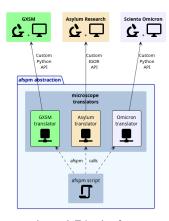


Code Reuse in SPM Scripting

Scripting with / without afspm

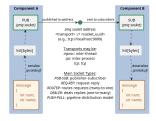


Code Reuse in SPM Scripting



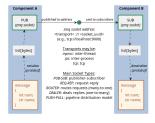
Approach Taken by afspm

Communication Protocol



Generic schemas sent between network sockets held by components.

Communication Protocol

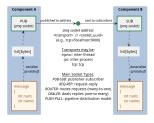


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Serialization / Deserialization

Translates data structures into a format that can be stored/communicated. Google Protocol Buffers: avoids schema violations, extra error handling.

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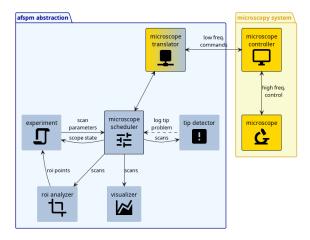
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Data Transmission Protocol

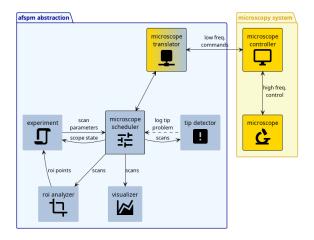
Handles sending of data between 'sockets' via common 'nodes'.

ZeroMQ: abstracts away transports used, handles common roadblocks.

Example



Example



- ROI Analyzer reviews scans for interesting regions.
- **Experiment** switches between scanning a large region or a suggested ROI.
- **Tip Detector** evaluates the state of the tip, logs problem if deemed poor.
- Visualizer visualizes what is being scanned.

Our publisher-subscriber, control-request world

We subscribe to events published by the SPM and request actions of it.

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- The SPM **publishes** messages types when its 'state' changes.
- Components may **subscribe** to only messages of interest.
- Messages may be **cached** by the Scheduler, to send to new components.

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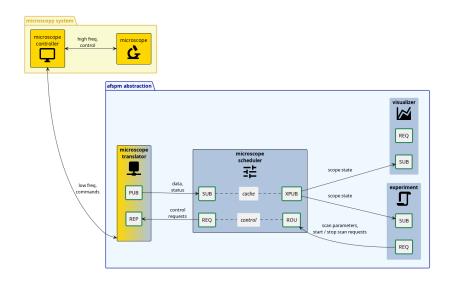
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Control Path

- Components send **requests** to the SPM and receive **responses**.
- The Scheduler **routes** control to the SPM (one component at a time).
- Components not in control may flag **problems** control is dropped.
 - A user may **manually** fix a problem and unflag the problem.
 - A component that **fixes** a flagged problem can grab control.

afspm: Detailed View



Publisher-Subscriber Path

```
message DataAspects {
  optional Size2u shape = 1;
  optional string units = 2;
}
message SpatialAspects {
  optional Rect2d roi = 1;
  optional string units = 2;
}
message ScanParameters2d {
  optional SpatialAspects spatial = 1;
  optional DataAspects data = 2;
}
```

2D Scan Parameters Schema

```
message Scan2d {
  optional ScanParameters2d params = 1;
  optional google.protobuf.Timestamp timestamp = 2;
  optional string channel = 3;
  optional string filename = 5;
  repeated double values = 4;
}
```

2D Scan Schema

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2D Scan Schema

2D Scan Parameters Schema

```
Frame 1
                          'Scan2d'
Frame 2
                        Scan2d Data
```

Envelope

Serialized Data Structure

Message Format

Control Path

```
enum ControlRequest {
   REQ_UNDEFINED = 0;
   REQ_ACTION = 1;
   REQ_PARAM = 2;  // [...]
   REQ_REQUEST_CTRL = 6;  // [...]
   REQ_ADD_EXP_PRBLM = 8;  // [...]
   REQ_SET_CONTROL_MODE = 10;
}
```

Control Request Schema

Control Response Schema

Design Particulars

Control Path

```
enum ControlRequest {
   REQ_UNDEFINED = 0;
   REQ_ACTION = 1;
   REQ_PARAM = 2;  // [...]
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   REQ_ADD_EXP_PRBLM = 8;  // [...]
   REQ_SET_CONTROL_MODE = 10;
}
```

Control Request Schema

```
enum ExperimentProblem {
   EP_NONE = 0;
   EP_TIP_SHAPE_CHANGED = 1;
   EP_DEVICE_MALFUNCTION = 2;
   EP_FEEDBACK_NON_OPTIMAL = 3;
}
```

Experiment Problem Schema

Control Response Schema

```
enum ControlMode {
   CM_UNDEFINED = 0;
   CM_MANUAL = 1;
   CM_AUTOMATED = 2;
}
```

Control Mode Schema

Control Path

```
enum ControlRequest {
 REQ_UNDEFINED = 0;
 REQ ACTION = 1:
 REQ_PARAM = 2; // [...]
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 REQ SET CONTROL MODE = 10:
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Control Request Schema

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enum ExperimentProblem {
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```

Experiment Problem Schema

```
Frame 1
                 REQ REQUEST CTRL
Frame 2
               EP_TIP_SHAPE_CHANGED
```

```
enum ControlResponse {
 REP SUCCESS = 0:
 REP_FAILURE = 1;
                       // [...]
 REP_NO_RESPONSE = 3;  // [...]
 REP_PARAM_NOT_SUPPORTED = 8; // [...]
```

Control Response Schema

```
enum ControlMode {
 CM_UNDEFINED = 0;
 CM MANUAL = 1:
 CM AUTOMATED = 2:
```

Control Mode Schema

```
Command Request Enum
Serialized Data Structure(s)
```

Message Format

Spawning, Monitoring, and the Config File

An experiment defined via a config file, with components spawned as needed.

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- Each component is instantiated as a child process (independent memory).
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- We can spawn different components on different computers.
 - The 'spawn' command allows indication of which components to spawn.

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Monitoring

- The parent process monitors spawned components for heartbeats.
- If a process has not 'beat' in a timeframe, it is killed and respawned.
- Then the caching logic chosen is important must be able to run.

Sample Config File

```
# --- URLs --- #
pub_url = "tcp://127.0.0.1:9000"
psc_url = "tcp://127.0.0.1:9001"
server_url = "tcp://127.0.0.1:6666"
router_url = "tcp://127.0.0.1:6667"
# [...]
exp_scan_res = [256, 256]
# [...]
```

```
# ---- PubSub ---- #
[translator.pub]
class = 'afspm.io.pubsub.publisher.Publisher'
url = 'pub_url'
# [...]
[experiment_sub]
class = 'afspm.io.pubsub.subscriber.Subscriber'
sub_url = 'psc_url'
# [...]
```

General Variables

Intermediary Classes

```
[translator]
component = true
class = 'afspm.components.microscope.translators.gxsm.translator.GxsmTranslator'
publisher = 'translator_pub'
control_server = 'translator_server'
# [...]
```

Config Components

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Operating Modes

- If switching between operating modes with presets, use actions.
- If needing to explicit parameters, add new 'composite' parameter request.

The End

Let us know what you think and help us make it better.

 $af spm\ on\ github$