Automated probe microscopy via evolutionary optimization at the atomic scale

9th Annual HUMIES Awards

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Julian Stirling, Adrian Radocea, Prof. Philip Moriarty, Prof. Natalio Krasnogor
The Power of Scanning Probe Microscopy

Imaging individual molecules and resolving sub molecular structure

The ability to fabricate electronic devices (a single atom transistor) with atomic precision.

The importance of the probe structure; a single H atom at the probe apex inverts the image contrast.
Scanning Tunneling Microscopy

Imaging parameters:
- Tunnel current, $i_t$
- Voltage, $V$
- Gain, $G$

\[ i_t \propto V \exp(-2kz_{ts}) \]

Where the tip-sample separation, $z_{ts}$, is maintained by a feedback loop of gain, $G$.

User parameters:
- $V$
- $i_t$
- $G$

Nanoscale:
- Tip apex
- Tunneling electrons
- Sample

Macroscopic scale:
- Actuator
- Probe or tip

Evolutionary optimization at the atomic scale
The problems:

• Changing tip state and,
• Obtaining the optimum imaging parameters $V$, $i$ and $G$

30 years without a solution, until now (Criteria E & G)

• Thousands of users world wide
• Expensive machine and operator costs
• Many hours spent manually optimising images
The cGA: An individual, $n$, with imaging parameters $V_n$, $i_n$ and $G_n$

The population of $N$ individuals, each with imaging parameters $V$, $i$, $G$

Fitness = RMI($T$, $I$)

Target Image, $T$

Acquired Image, $I$

The cGA in operation

(Criteria F)

- Images taken by microscope for the individual’s parameters V, i, G
- Migrate good V, i, G

Generation vs. Fitness

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Can we choose different tip states?

(Techniques E & D)

Is it comparable to the human operator?

(Criteria H)

Results of the challenge

<table>
<thead>
<tr>
<th>Microscopist</th>
<th>Average image quality</th>
<th>Change in image quality per min</th>
</tr>
</thead>
<tbody>
<tr>
<td>Machine</td>
<td>0.20*</td>
<td>7.1*</td>
</tr>
<tr>
<td>Human</td>
<td>0.09</td>
<td>2.6</td>
</tr>
</tbody>
</table>

*winner

A selection of the machine optimised images:

The Competition (Human vs. Machine):
Obtain the best image possible within 1 hour

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Criteria for human-competitiveness

(A) The result was patented as an invention in the past, is an improvement over a patented invention, or would qualify today as a patentable new invention

- New invention
- Working with the leading manufacturer

(D) The result is publishable in its own right as a new scientific result independent of the fact in was mechanically created.

- The same journal as the original Nobel prize winning invention

(E) result $\geq$ the most recent human-created solution to a long-standing problem for which there has been a succession of increasingly better human-created solutions.

- The human operator was the solution
Criteria for human-competitiveness

(F) result $\geq$ a result that was considered an achievement in its field at the time it was first discovered.

• The system is state of the art

(G) The result solves a problem of indisputable difficulty in its field.

• “That’s impossible”
• “Can we have it, please?”

(H) The result holds its own or wins a regulated competition involving human contestants (in the form of either live human players or human-written computer programs)

• The ‘Nano-machine’ won!
Summarising why this entry is best!

- A step-wise change in STM operation for over 30 years
- An underpinning technology for the wider scanning probe instrumentation sector
- Innovative
- Greatly improved productivity
- State of the art
- Meets 6 out of the 8 criterion

It’s just the tip of the iceberg....
What does the future hold for a robot that can recognise atoms and molecules...

....and can develop the nanoscale tools and necessary protocols to manipulate those atoms and molecules?

What would you get the robot to build?

What if it evolved things that it wanted to?
The authors would like to thank the EPSRC (Grant no: EP/H010432/1) and the European Commission’s ICT-FET programme via the Atomic Scale and Single Molecule Logic gate Technologies (AtMol) project, Contract No. 270028 for providing financial support to this project.