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The Future of Crystallographic Computing



Scientific software – meaning...?

- **How relevant will your work be in 20 years?**
- Software needs a lot to persist (curation, user acceptance, portability, easy installation and maintenance etc)
- Does good methods development need a scientific discovery?

What motivates us to write crystallographic software?

(Answers please!)

Scientific programmer or programming scientist?

Durability of impact



algorithm

method

library

software

GUI

distribution

Programming scientist:

- Old computation/algorithms
- Experimental knowledge
- Algorithms from other fields

For the scientific programmer:

- Hardware
- Broad knowledge of software development
- More direct user contact

Survey

Which crystallographic discipline?

- 12 Macromolecular Crystallography
- 11 Small Molecules
- 5 Powder
- 2 ED
- 2 XFEL
- 2 Hardware
- 0 Mineralogy
- 1 Magnetism

Survey

	Chemist	Biologist	Physicist	Mathe- matician	Computer Scientist	Other
Over 50	3		3			
Over 40	2		1			
Over 30	2		4			
Younger		3	2			3

Automation

High level with automation and graphic user interfaces:
Crystallography becomes very accessible.

This is a good thing!

- But it means we write software for an inexpert audience.
- It also means that we often teach methods alongside with our software.

“The software developer, the teacher of the nation.”

This makes us a good field for the extroverted programmer.
Or the introverted programmer with an extroverted friend...

Assorted computational challenges

Powder?

Mineralogy?

SAXS?

Diffuse scatter?

Small molecule crystallography

- Service crystallography; software is taken for granted
- Crystal structure design
- Strong interactions with computational chemistry

Macromolecular crystallography

- Ever more automation
- Structure numbers grow exponentially, but big data studies few

Serial data & XFEL

- Very big data sets
- New software for mainly for integration and diagnosis
- Sources of error?

Assorted computational challenges

Neutron scattering

- Laue data difficult to integrate
- Dedicated integration/Scaling for macromolecular data
- These are not X-ray data!


Electron diffraction

- Natural realm of very small crystals - MicroED
- Diffraction geometry (astigmatism/focus change during collection)
- These are not X-ray data!

Single-particle Cryo-EM:

- Now up to 2Å, modelling with X-ray crystallographic tools
- These are not X-ray data!
- Industrial applications?

Datapocalypse

A close-up photograph of a yellow fire hydrant. Water is being sprayed from the side outlet, creating a large, white, turbulent plume that fills the right side of the frame. The background is dark, making the yellow hydrant and the white water stand out.

Getting **a structure** off the
XFEL is like taking a
drink from a fire hydrant.

Mitchell Kapor

Datapocalypse

Users today are collecting lots of data. Most of which is...

- bad quality
- problematic
- And they will never use...
- **How to guide collection in a better way?**
- **How to select what to store? (Machine learning?)**
- **How to store?**
 - > **Data base design?**

Derived objectives for this Forum:

Look for the science in crystallographic computing!

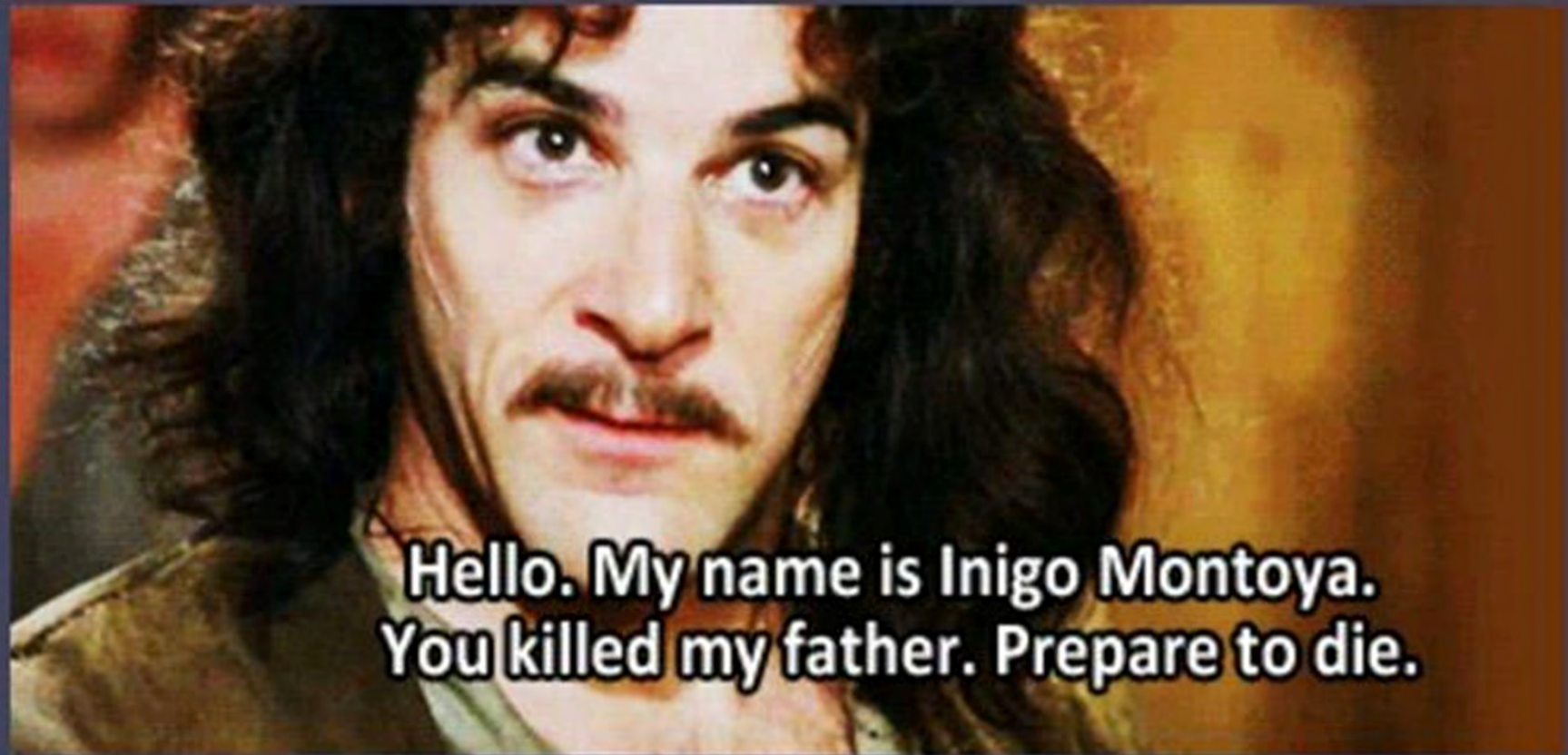
If you do not think it's **interesting**, don't do it— it might not be science, useful or fulfilling.

 **crystallography**

Ask, and if you do not understand the answer, ask again.
(This includes lecturers.)

Networking: Here you can meet your peers, other generations of programmers, and people who do similar things but are from different fields. **Be curious.**

How to introduce yourself



Remember Inigo Montoya:

1. Polite greeting
2. Name
3. Relevant personal link
4. Manage expectations

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Have fun!

Conclusion

What's past is prologue.

- Shakespeare, The Tempest