First Steps in Scientific Programming

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Overview

- Where to start
- The learning curve
- Elements of a computer
- The “terminal”, CL, UNIX tools
- Concepts of programming irrespective of language, code optimisation
- Thinking big and long term
- Miscellaneous issues

Where to start: the audience

- Young (inexperienced) scientists or science/engineering students
- Limited exposure to programming
- Eager to learn (or not)
- Pressured to produce ASAP
- “Land” in projects, 0-input on choices
- In their future, they will lead projects involving computers, programming decisions and acquisition of resources

The learning curve

- The environment, how to do things in a computer
- What “things” you can do
- How to make these things to happen
- How to organise information
- Forget spreadsheets, this is “the real word”
- The available tools, OS, languages, different architectures
- What to learn (???)

Main computer components

- Not just a magical box, everything below is finite

- Hardware:

1. The processor(s): CPU, GPU

2. The storage components

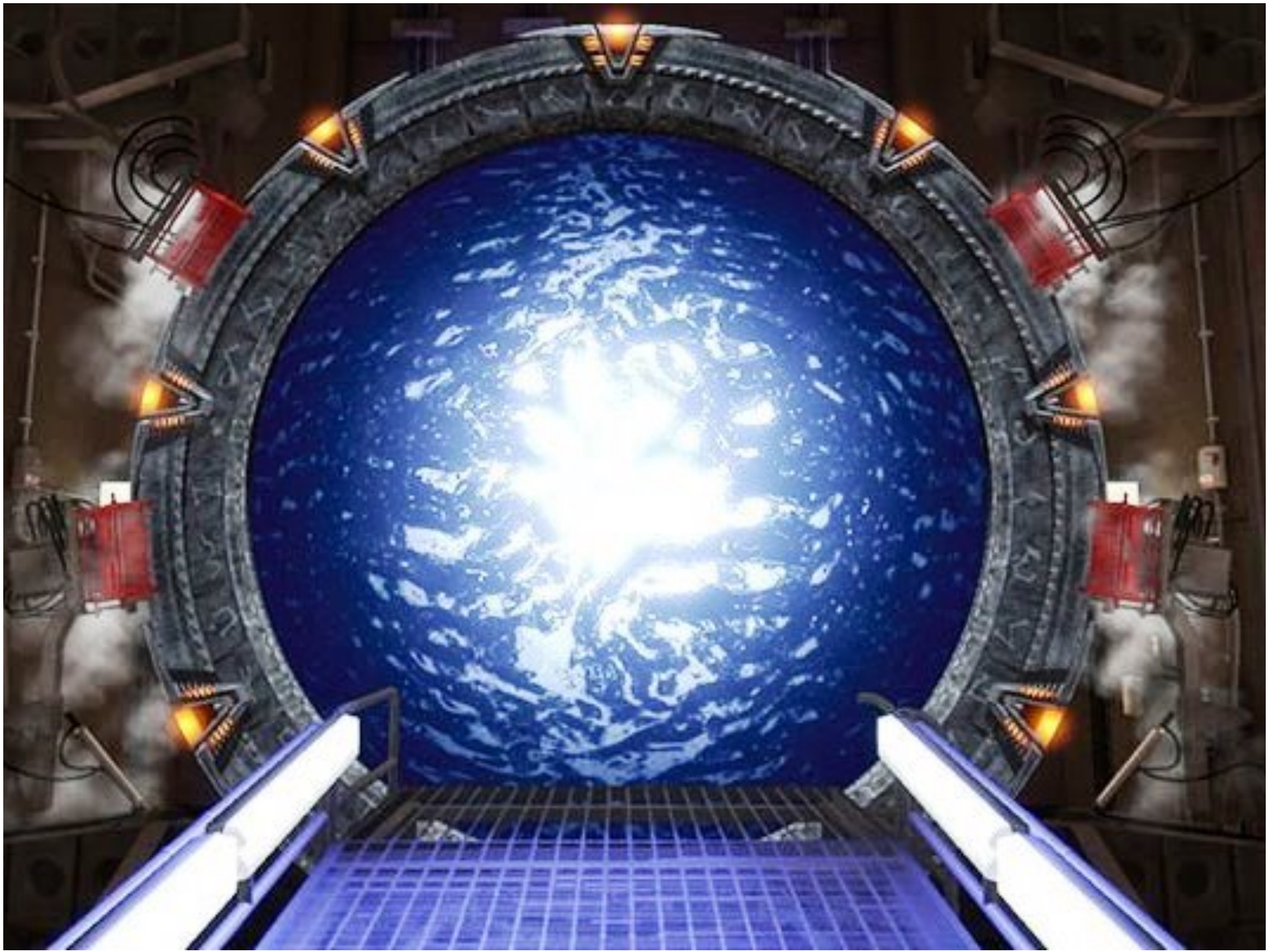
3. Memory

- Software:

A. Programming languages, compilers, interpreters

B. Special libraries, text editors, apps, paths, ETC.

The terminal



The terminal

- A psychological barrier for millennials. It needs demystifying
- Command line (!GUI), but real power if embraced
- UNIX: Microsoft ❤️ Linux. Future of the cloud, IOT
- Plenty of tools that save you from programming:
  - Man, ls, head, tail, find, awk, grep, ps, shells, sed, mv, cp, od
  - Remote work: ssh, scp, sftp, rsync
  - Versioning: SVN, git
  - Editing: vim, emacs, nano, textwrangler, ETC. Personal preference
  - Typesetting: tex and family, open-office, ETC.

Elements of programming

- Variables
- Objects
- Sub-programs / methods (variable scope)
- Flow control: conditionals, loops, exception
- Demo code, prototypes, production code
- Low data-volume v high data-volume
- Systematic Code testing

Code optimisation

- Code optimisers do exist, but they do not replace good programming practices and they may introduce undesired “features”
- Consider using look-up tables
- Some operations are really “expensive”, avoid them. (pow, exponentials, trigonometric, polynomials).
- Learn about existing libraries, avoid reinventing the wheel
- Manage memory well, whatever variable/object created occupies space. Beware of memory leaks.
- Be aware of overheads

Prepare for the long run

- Longevity of code
- Longevity of data
- Use adequate data characterisation/description for sharing
- Good practices to share data
- If data volume is significant, store in binary. Binary is the natural way for a computer to store information, human readable format is not.
- Whenever possible, add uncertainty information to your data. Somebody might want to run a model using your data.

Miscellaneous issues

- Things do fail, ergo, learn how to fix (debug) ASAP
- Even your computer can fail. Backup, better, user versioning
- Learn about “accelerators” (TAB key, use of make, ETC)
- Learn to profile your code (memory, exec-time, IO, etc.)
- When all else fails, ask for help, but write a clear description of the problem “It doesn’t work” is not enough.
- Learn how to alter someone else’s code effectively
- Plan your programs as if they were projects, learn about flowcharts, use pseudo coding, try thinking of different scenarios.
- Learn to handle time and time dependent situations.