Matching Research Requirements to Software

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Write your own OR Use existing?

- Writing your own software
  - Don’t reinvent the wheel!
    - Do a survey on what’s available
    - Use existing libraries (LAPACK, etc.) and solvers
    - Modify / improve / reuse existing codes / routines
  - Use best practices
    - Version control (git)
    - Document, document, document!
    - Leave room for improvements / change of methods (reviewer requests for example)
• Writing your own software ...

  – Testing
    • Unit testing (testing individual units)
    • Regression testing (testing overall functionality)

  – Verification
    • Compare numerical results with analytical solutions
    • Compare with other published results
    • Run benchmark tests
Use Community Software

• Find commonly used in your research area
  – Publications / other researchers / friends

• Well documented
  – Manuals
  – Peer reviewed publications

• Evaluate usability
  – Does it fit the needs
  – Special hardware or software (libraries/compilers) needs

• Check accuracy
• Use Community Software …
  – Benchmarks (some packages provide benchmarks ready to run)
    • Tests for performance and scalability in a cluster environment
  – Currently being developed and supported
    • Stable versions, no alpha, beta releases!
    • “User friendly” developer or not