James C. Phillips
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• Background:
  • Ph.D. in Physics (theoretical and computational biophysics)
  • 1999-2017 lead developer of NAMD molecular dynamics software
  • Implemented or guided implementation of many methods
  • Various techniques to simplify coding in Charm++:
    • Cooperative threads with suspend/resume
    • Structured programming of message-driven execution
    • Top-level and embedded scripting (Tcl and Python)

• Philosophical motivation:
  • Software is the precise and testable expression of theory.
  • Theory is the abstract and untestable description of software.
  • Scientific assertions must be testable/falsifiable by experiment.
  • Hence theory cannot be science without software.
Research vs Production Codes

• Research Codes
  • Used to develop and test methods
  • Designed/evolved to be easy to modify (at least by the original author)
  • May ignore corner cases, only handle small test-cases

• Production Codes
  • Used perform actual domain science
  • Designed/evolved for performance and reliability
  • Needs to serve many users, run on full-scale science models

• Issues due to separation
  • Research codes come and go, effort is repeated and lost
  • Methods are never migrated to production code or tested at scale
  • Now focus on building portable user-extensibility into production code