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Theory-Software Translation Workshop - US Edition in New Orleans, LA (February 4-5, 2019)

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Supercomputing Applications

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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