Trilinos Software Engineering Technologies and Integration

2008-7718P

- Numerical Algorithm Interoperability and Vertical Integration
  - Abstract Numerical Algorithms (ANAs)
  - Thyra (Interoperability and vertical integration of ANAs)
  - Epetra (Interoperability of element-based numerical algorithms)
- General Software Interoperability and Integration
  - Memory management (Teuchos::RCP, ...)
  - User input and configuration control (Teuchos::ParameterList, ...)
  - User introspection (Teuchos::FancyOStream, ...)
- Skin packages (wrappers for other languages)
  - PyTrilinos
  - ForTrilinos
- General Software Quality and Design
- Lean/Agile Software Engineering Principles and Practices
  - Internal Trilinos issues
  - External customer issues

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Trilinos Strategic Goals

- **Scalable Computations:** As problem size and processor counts increase, the cost of the computation will remain nearly fixed.
- **Hardened Computations:** Never fail unless problem essentially intractable, in which case we diagnose and inform the user why the problem fails and provide a reliable measure of error.
- **Full Vertical Coverage:** Provide leading edge enabling technologies through the entire technical application software stack: from problem construction, solution, analysis and optimization.

Algorithmic Goals

- ***Grand* Universal Interoperability**: All Trilinos packages will be interoperable, so that any combination of solver packages that makes sense algorithmically will be possible within Trilinos.

Thyra is being developed to address this issue

- **Universal Accessibility:** All Trilinos capabilities will be available to users of major computing environments: C++, Fortran, Python and the Web, and from the desktop to the latest scalable systems.
- **Universal Solver RAS**: Trilinos will be:
  - Reliable: Leading edge hardened, scalable solutions for each of these applications
  - Available: Integrated into every major application at Sandia
  - Serviceable: Easy to maintain and upgrade within the application environment.

Software Goals

Courtesy of Mike Heroux, Trilinos Project Leader

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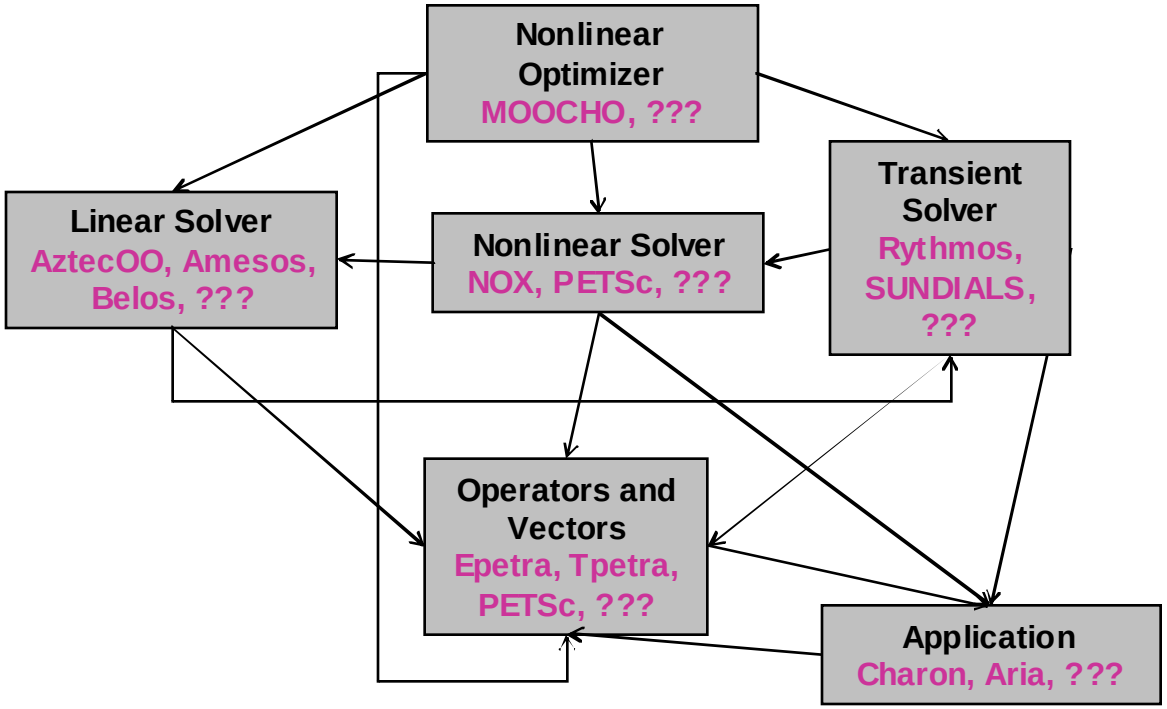
Algorithm Vertical Integration for Embedded Algorithms

Example: Numerous interactions exist between layers of abstract numerical algorithms (ANAs) in a transient optimization problem



What is needed to solve problem?

- Standard interfaces to break $O(N^2)$ 1-to-1 couplings

Thyra is being developed to address interoperability of ANAs by defining interfaces for:

- Linear operators/vectors
- Preconditioners / Linear solvers
- Nonlinear models
- Nonlinear solvers
- Transient solvers

Key Points

- Higher level algorithms, like optimization, require a lot of interoperability
- Interoperability and vertical integration must be “easy” or these configurations will not be achieved in practice

General Software Interoperability and Integration

- Memory management
  - Replace all raw C++ pointers in all higher level C++ code
  - Single objects: Teuchos::RCP, Teuchos::Ptr,
  - Arrays of objects: Teuchos::Array, Teuchos::ArrayRCP, Teuchos::ArrayView, ...
- User input and configuration control
  - Teuchos::ParameterList:
    - General parameter database
    - Self documenting
    - Validation support
    - XML input and output
  - Teuchos::ParameterListAcceptor:
    - Standard interface & protocal for handling ParameterList
- User introspection
  - Teuchos::FancyOStream
    - Formatted nested output
  - Teuchos::Describable
    - Flexible output of the state of an object
  - Teuchos::VerboseObject
    - Output showing dynamic behavior of an object
  - Teuchos::TimeMonitor
    - Targeted timing of critical computations and performance monitoring

Lean/Agile Software Engineering Principles and Practices

- Internal Trilinos development tools principles and practices
  - Scalability and robustness of build system and test tools
  - Continuous integration development principles and practices
  - Release process principles and practices

- Integration with customer application codes
  - Coordination of co-development with customer application codes (i.e. daily integration and asynchronous continuous integration)
  - Coordination of release schedules with customer application codes

Trilinos Software Engineering Capabilities Area Webpage

http://trilinos.sandia.gov/capability_areas.html