PyTrilinos: A Python Interface to Trilinos

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Sandia National Laboratories

Reproducible Research in
Computational Geophysics
August 31, 2006

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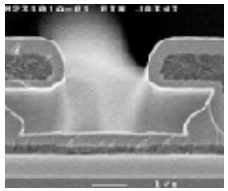
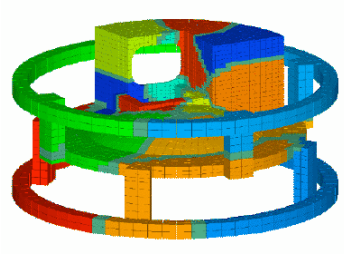
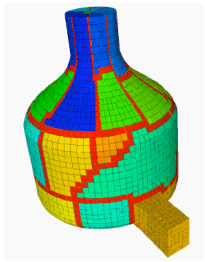
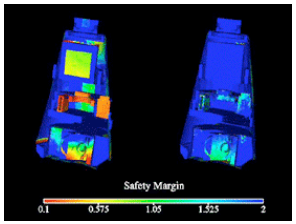
Computational Sciences at Sandia



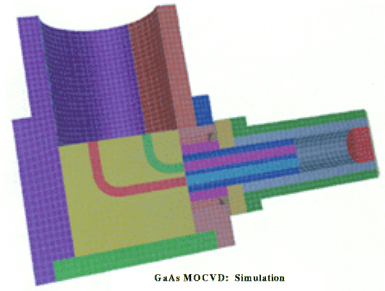


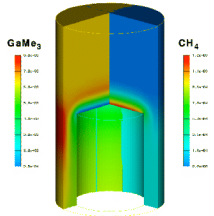


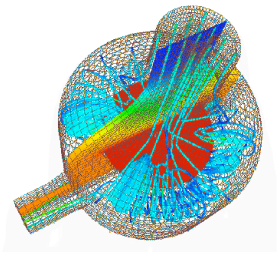


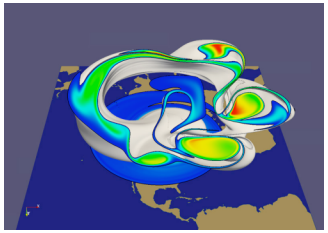
- Chemically reacting flows
- Climate modeling
- Combustion
- Compressible flows
- Computational biology
- Electrical modeling
- Heat transfer
- Load balancing

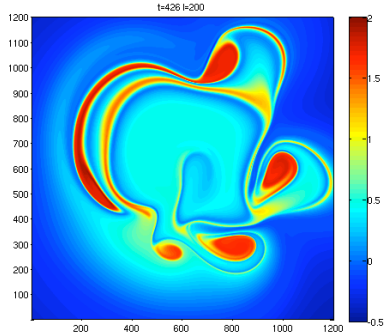
- Materials modeling
- MEMS modeling
- Mesh generation
- Optimization and uncertainty quantification
- Seismic imaging
- Shock and multiphysics
- Structural dynamics

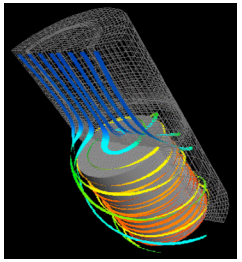


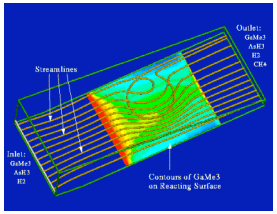


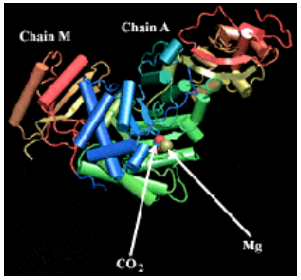




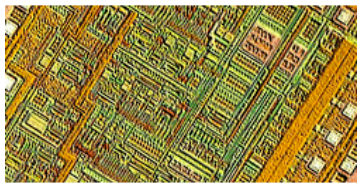








MDL ASICS



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The Trilinos Project

- Provide a central repository for Sandia's solver technology
- Increase code-reuse
- Organized on concept of "packages"
- Minimize package interdependence
- Maximize package interoperability
- Provide a framework for SQE and SQA
  - Compliance with requirements
  - Nightly test harness
- High degree of developer autonomy
- Open source: GNU Lesser License
- Web site: http://software.sandia.gov/trilinos
- Next release: Version 7.0, September, 2006
- Trilinos Users Group Meeting, November 7-9, 2006

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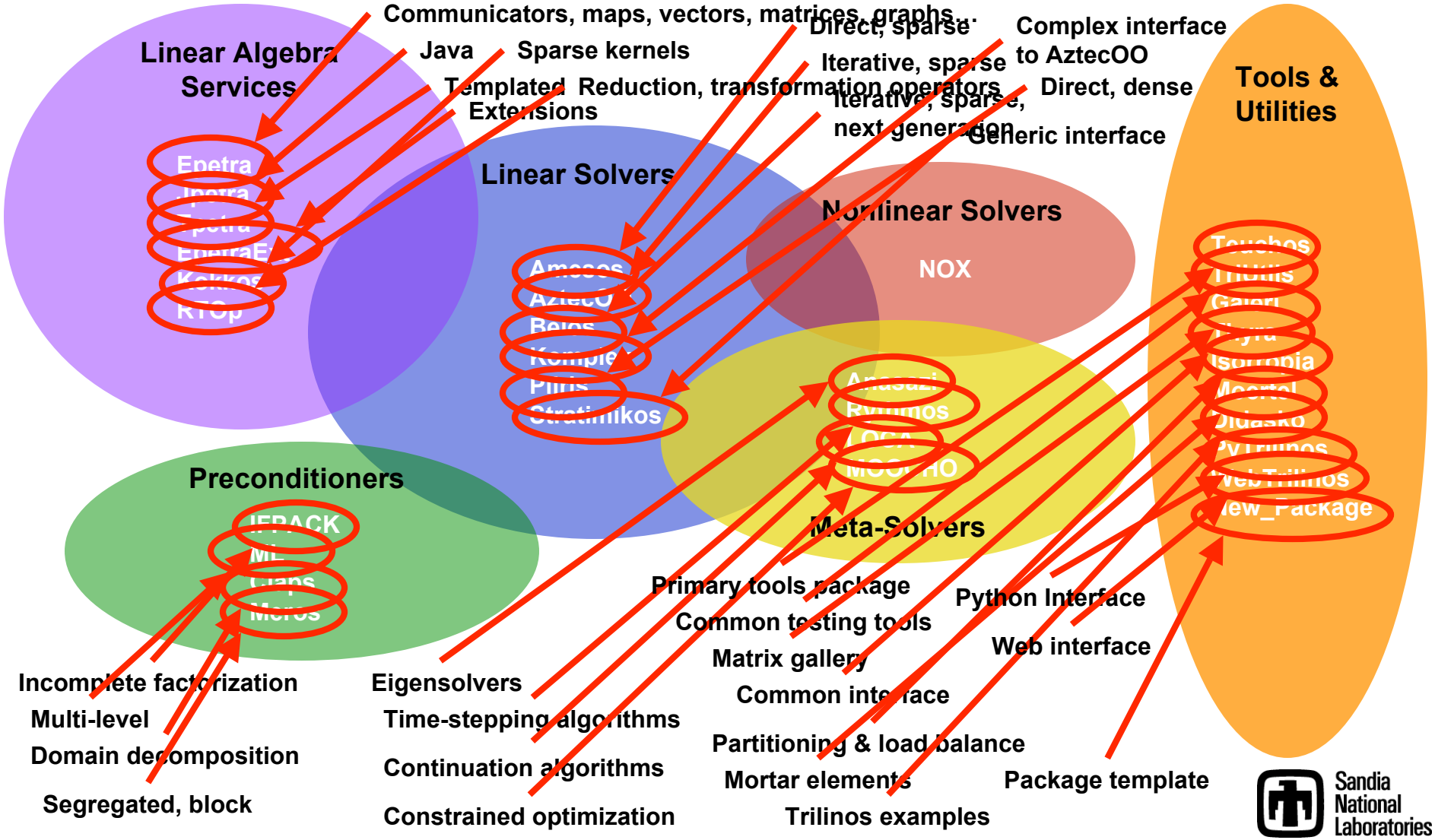
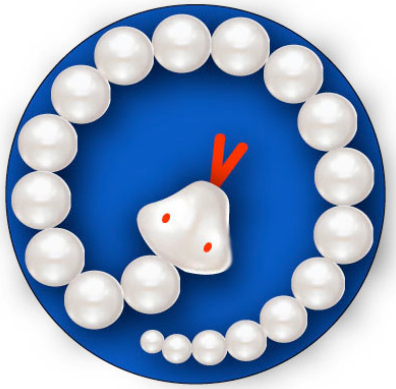


The Interoperability Problem

- Ross has talked about the need for (and work on) a common abstract interface
  - Interfaces between Trilinos packages
  - Interfaces between Trilinos and external packages
- We would like to extend this concept to the python wrappers
  - Interoperability with external python projects, such as SLIMpy
  - Many design decisions still to be made
  - Some early prototyping work has been done

PyTrilinos



- **Linear Algebra Services**
  - **Epetra** (with extensive NumPy compatibility and integration)
  - **EpetraExt** (coloring algorithms and some I/O)
- **Linear Solvers**
  - **Amesos** (LAPACK, KLU, UMFPACK, ScaLAPACK, SuperLU, SuperLUDist, DSCPACK, MUMPS)
  - **AztecOO**
- **Preconditioners**
  - **IFPACK**
  - **ML**
- **Nonlinear Solvers**
  - **NOX** (python wrappers not yet caught up to recent redesigns)
- **Meta-Solvers**
  - **LOCA** (python wrappers not yet caught up to recent redesigns)
  - **Anasazi** (early development stage)
- **Tools and Utilities**
  - **Teuchos** (ParameterList class only)
  - **TriUtils**
  - **Galeri**
  - **Thyra** (early development stage)
  - **New_Package**

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PyTrilinos Documentation

- Trilinos documentation is handled by `doxygen`: special comments within code
  - Web pages updated twice daily
- Python wrappers are generated using `swig` … `doxygen` does not work with swig interface files
  - %feature("autodoc", "1");

```
>>> help(Epetra.Vector.Dot)
  Dot(*args) unbound PyTrilinos.Epetra.Vector method
    Dot(self, Epetra_Vector A) -> double
```

- Currently working to provide much more extensive documentation highlighting differences between C++ and python interfaces
  - Release 7.0 in September

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PyTrilinos.Epetra

- Communicators
  - `Comm`
  - `SerialComm`
  - `MpiComm`
  - `PyComm`
- Maps
  - `BlockMap`
  - `Map`
  - `LocalMap`
- Vectors
  - `MultiVector`
  - `Vector`
  - `IntVector`
- SerialDense objects
  - `SerialDenseOperator`
  - `SerialDenseMatrix`
  - `SerialDenseVector`
  - `SerialDenseSolver`
  - `IntSerialDenseMatrix`
  - `IntSerialDenseVector`
- Graphs
  - `CrsGraph`
- Operators
  - `Operator`
  - `RowMatrix`
  - `CrsMatrix`

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A Quick Detour…

- Python lists are not suitable for scientific computing
  - Flexible but inefficient
  - Heterogeneous data, noncontiguous memory
- NumPy module provides needed functionality
  - Contiguous, homogeneous n-dimensional arrays
  - High-level interface
  - Part of SciPy
- SciPy is a large, open source package for a wide variety of python interfaces to scientific software:
  - NetLib's "greatest hits"

PyTrilinos.Epetra and NumPy

- Array-like classes inherit from `numpy.UserArray`
  - `MultiVector`
  - `Vector`
  - `IntVector`
  - `SerialDenseMatrix`
  - `SerialDenseVector`
  - `IntSerialDenseMatrix`
  - `IntSerialDenseVector`
- Methods throughout Epetra have arguments that accept or produce pointers to C arrays
  - Python input arguments accept python sequences
  - Python output arguments produce `ndarrays`

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PyTrilinos.Teuchos

- Teuchos::ParameterList
  - Used by several Trilinos packages to set problem parameters
  - Maps string names to arbitrary-type values
  - Python implementation allows dictionary substitutions
  - Hybrid PyDictParameterList objects are returned
  - The following conversions are supported:

Python	Dir	C / C++
`bool`	⇔	`bool`
`int`	⇔	`int`
`float`	⇔	`double`
`string`	⇔	`std::string`
`string`	⇐	`char *`
`dict`	⇒	`ParameterList`
wrapped `ParameterList`	⇔	`ParameterList`
wrapped `PyDictParameterList`	⇒	`ParameterList`

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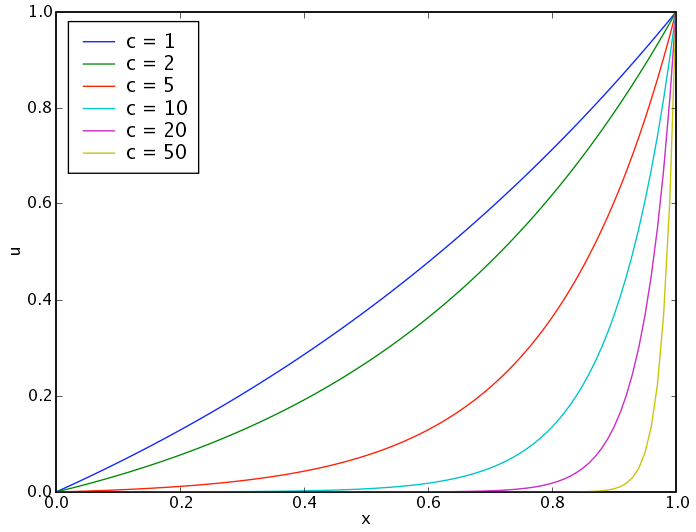
PyTrilinos Demonstration

- **Governing equation:** $-\frac{d^2u}{dx^2} + c\frac{du}{dx} = 0, \quad x \in [0,1]$
- **Boundary conditions:** $u(0) = 0, \quad u(1) = 1$
- **Exact solution:** $u(x) = \frac{e^{cx} - 1}{e^c - 1}$
- **CDS:** $-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + c\frac{u_{i+1} - u_{i-1}}{2h} = 0$
- **Oscillations:** $ch = \frac{c}{n-1} > 2$



Conclusions

- Python lets developers focus on the problem
  - Memory management, garbage collection
  - Powerful, flexible containers
  - Clean, readable syntax
- PyTrilinos provides access to powerful solver technologies
  - Rapid prototyping
  - Application development
- For computational geophysics, Thyra should provide key too interoperability
  - Python wrappers for Thyra
  - Thyra adapters for geophysics codes

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