Parallel PDE Solvers in Python

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Sandia National Laboratories

Scientific Python 2006
August 18, 2006

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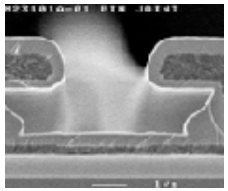
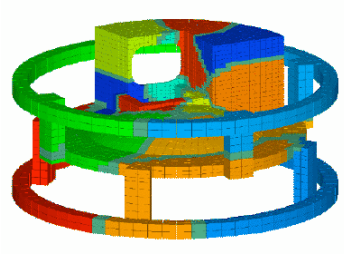
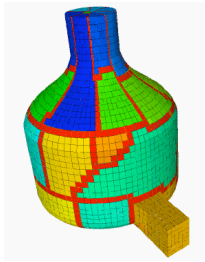
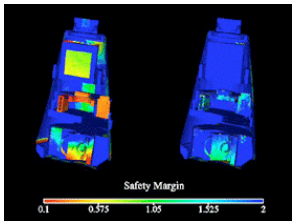
Computational Sciences at Sandia



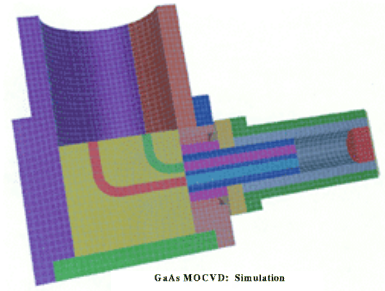


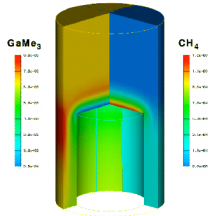


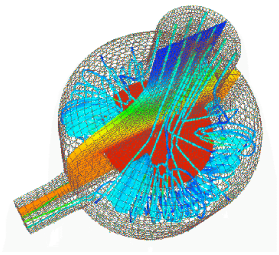


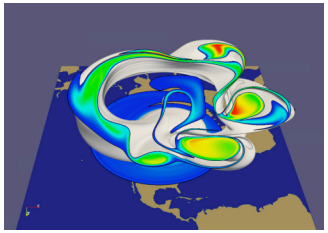
- Chemically reacting flows
- Climate modeling
- Combustion
- Compressible flows
- Computational biology
- Electrical modeling
- Heat transfer
- Load balancing

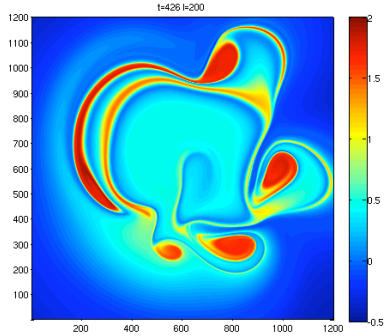
- Materials modeling
- MEMS modeling
- Mesh generation
- Optimization and uncertainty quantification
- Seismic imaging
- Shock and multiphysics
- Structural dynamics

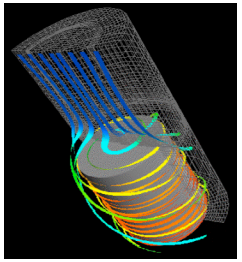


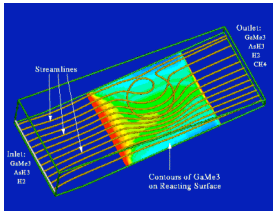


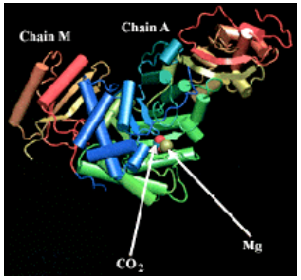




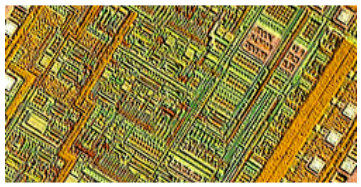








MDL ASICS



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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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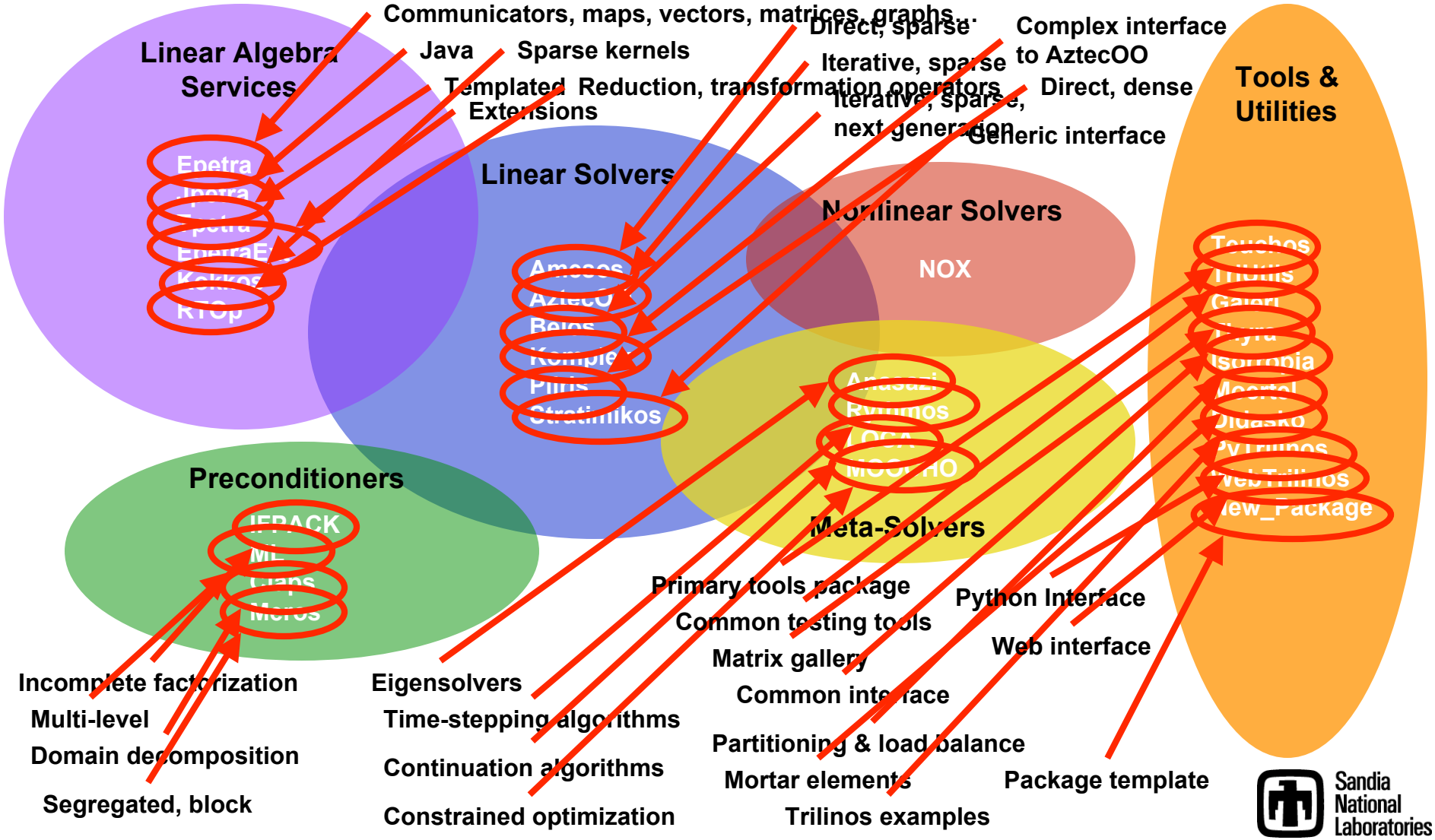
The Trilinos Project



The Interoperability Problem

- ~20 “core” packages → ~400 interface package boundaries
- The purpose of the Thyra package is to provide tools and definitions for a common interface
  - Packages that code to the interface should be able to interact with each other
  - Important, but relatively new effort within Trilinos (replacing TSF):
    - Thyra
    - RTOp
    - Stratimikos
    - Rythmos
    - …
  - SciDAC TOPS proposal: universal operability
  - Actively pursuing funding for python implementation of Thyra (some prototyping done)

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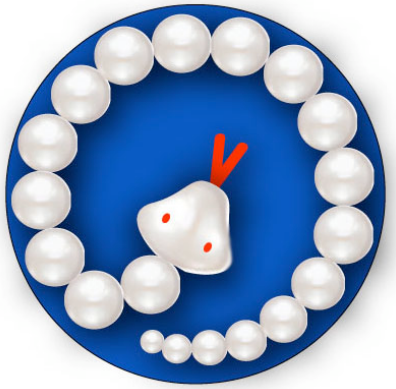
PyTrilinos



- **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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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:** $ch = \frac{c}{n-1} > 2$