PyTrilinos: A Parallel Python Interface to Trilinos

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Trilinos Packages

Linear Algebra Services	Epetra	Kokkos	Komplex	
Linear Solvers	AztecOO	Amesos	Pliris	Belos
Preconditioners	IFPACK	ML	Claps	Meros
Eigensolvers	Anasazi			
Nonlinear Solvers	NOX			
Continuation Algorithms	LOCA			
Abstract Interfaces	Thyra	TSFCore	TSFCoreUtils	TSFExtended
Utilities	Teuchos	EpetraExt	Triutils	Didasko

▨ = Next-Generation

PyTrilinos

What is PyTrilinos?

- PyTrilinos is a python interface to selected Trilinos packages
- What packages are wrapped?
  - Epetra, EpetraExt, Triutils, Galeri, AztecOO, Amesos, IFPACK, ML, New_Package
  - Outdated: NOX, LOCA
  - Early stages: Anasazi, Thyra
- Is MPI supported?
  - Yes, it is currently embedded in the Epetra module if Trilinos is configured with `--enable-mpi`

Scripting Interfaces

- Why add a scripting interface to Trilinos?
  - Interactive creation, manipulation and use of Trilinos objects without compilation step → rapid prototyping
  - Application development: scripting languages are good for command-and-control code that can hand off to compiled numerical kernels
- Why python?
  - Python was built from the ground up to be object oriented → maps directly to Trilinos design
  - Python was designed to be a teaching language → clean, readable syntax
  - Massive library of standard and third-party modules
  - Large and growing scientific python community

What About SciPy/Numeric (NumPy)?

- SciPy is a huge collection of wrappers for scientific libraries
- Most SciPy packages require multi-dimensional array objects to work on → Numeric (currently migrating to NumPy)
- SciPy's biggest omission is PDE solvers (sparse systems, parallel distributed data, and solvers that can use them)
- PyTrilinos is filling these gaps
- Certain Epetra classes overlap Numeric functionality (e.g. Epetra_MultiVector)
  - Python implementation of these classes inherit from both the Epetra class and Numeric arrays

Building & Installing PyTrilinos

- Prerequisites include python 2.3, Numeric, and swig (Simple Wrapper Interface Generator) 1.3.23
  - Swig is the workhorse for generating wrapper code; wrapper code is not pre-generated because of configuration options
- Add `--enable-python` to invocation of `configure`
- Python modules will be built for those packages that support it

Demonstration

PyTrilinos Performance vs MATLAB

- CPU sec to fill nxn dense matrix

n	MATLAB	PyTrilinos
10	0.00001	0.000416
100	0.0025	0.0357
1000	0.0478	3.857

- CPU sec to fill nxn diagonal matrix

n	MATLAB	PyTrilinos
10	0.00006	0.000159
1000	0.00397	0.0059
10,000	0.449	0.060
50,000	11.05	0.313
100,000	50.98	0.603

- CPU sec for 100 MatVecs

n	MATLAB	PyTrilinos
50	0.02	0.0053
100	0.110	0.0288
500	3.130	1.782
1000	12.720	7.150

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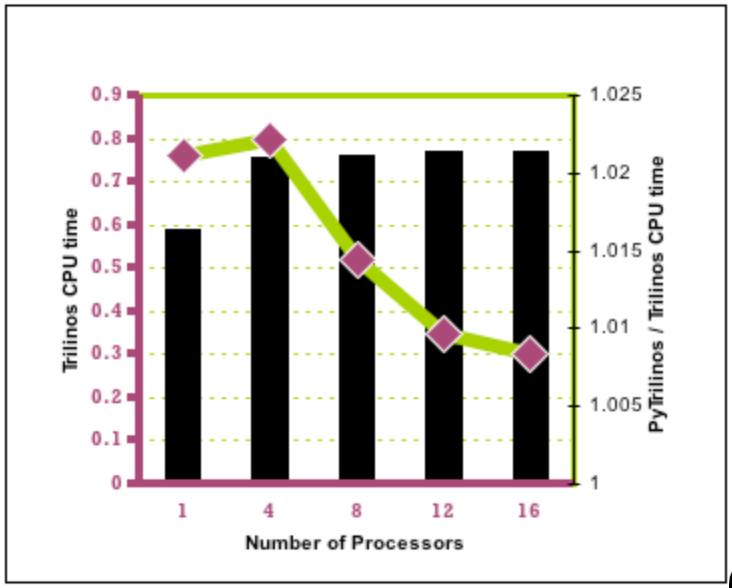
PyTrilinos Performance vs Trilinos

- Fine-grained script:

n	Trilinos	PyTrilinos
1000	0.010	0.15
10,000	0.113	0.241
100,000	0.280	1.238
1,000,000	1.925	11.28

- Course-grained script:



PyTrilinos Performance

- Some Trilinos packages are designed for users to derive classes from pure virtual base classes
  - Epetra_Operator
  - Epetra_RowMatrix
  - NOX::Abstract::Interface . . .
- Numerical kernels (matvecs, nonlinear function evaluations) are therefore written by users
- Using PyTrilinos, numerical kernels are therefore written in python (fine-grained . . . bad)
- If efficiency is a consideration,
  - Use array slice syntax
  - Use `weave`
  - Inefficient code is 20-100x slower

Summary

- PyTrilinos provides python access to selected Trilinos packages
  - Emerging from early stages . . . portability, completeness
  - Parallelism
  - Rapid prototyping
  - Application development
  - Unit testing
  - Numeric compatibility (migrating to NumPy)
- PyTrilinos complements and supplements the SciPy package