PDE Simulation with Python

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Organization

- PETSc Introduction
- Structural Considerations
- Implementations
- Future Directions

What is PETSc?

- A freely available and supported research code
  - Download from http://www.mcs.anl.gov/petsc
  - Free for everyone, including industrial users
  - Hyperlinked manual, examples, and manual pages for all routines
  - Hundreds of tutorial-style examples
  - Support via email: petsc-maint@mcs.anl.gov
  - Usable from C, C++, Fortran 77/90, and Python

What is PETSc?

- Portable to any parallel system supporting MPI, including:
  - Tightly coupled systems

    Cray T3E, SGI Origin, IBM SP, HP 9000, Sub Enterprise
  - Loosely coupled systems, such as networks of workstations

    Compaq,HP, IBM, SGI, Sun, PCs running Linux or Windows
- PETSc History
  - Begun September 1991
  - Over 8,500 downloads since 1995 (version 2), currently 250 per month
- PETSc Funding and Support
  - Department of Energy

    SciDAC, MICS Program
  - National Science Foundation

    CIG, CISE, Multidisciplinary Challenge Program

The PETSc Team


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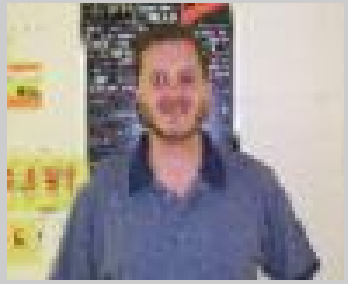
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Who Uses PETSc?

- Computational Scientists
  - PyLith (TECTON), Underworld, Columbia group
- Algorithm Developers
  - Iterative methods researchers
- Package Developers
  - SLEPc, TAO, MagPar, StGermain

Automatic Downloads

- Starting in 2.2.1, some packages are automatically
  - Downloaded
  - Configured and Built (in `$PETSC_DIR/externalpackages`)
  - Installed in PETSc
- Currently works for
  - PETSc documentation utilities (Sowing, lgrind, c2html)
  - BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
  - MPICH, MPE, LAM
  - ParMetis, Chaco, Jostle, Party, Scotch
  - MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack
  - Prometheus, HYPRE, ML, SPAI
  - Sundials

Structure of Scalable PDE Algorithms

Hierarchy

The central feature of algorithms for PDEs is

hierarchical decomposition

- Key operations
  - Restriction
  - Assembly
- Bulk of the computation is local

http://www.mcs.anl.gov/petsc/petsc-as/documentation/tutorials/sieve.pdf

Algorithms

- Multigrid
- FMM
- Finite elements
- Finite difference
- PETSc DA parallelism

Implications

Python for control and logic

C for local computation

- Decouple organization of storage from mathematical operations
  - Vectors are **not** arrays
- Lots of small arrays
  - `get/setValues()` methods
- Views into larger arrays
- Dense, local computation is cache/bandwidth efficient

Wrapper Implementations

Implementations

- PETSc (SIDL)
  - Parsers a SIDL interface description
  - Generates a C extension module for each class and Python for enums
- petsc4py (SWIG)
  - Lisandro Dalcin (CIMEC)
  - Parsers headers
  - Generates a single C extension module and Python for each class
- pypetsc (Pyrex)
  - Simon Burton (ANU)
  - Parsers headers
  - Generates a single C extensions module and Python infrastructure
  - Python handles initialization/finalization and creation/destruction

Commonalities

Interface is more important than implementation

- Class and method names
  - Type signatures
  - Function pointer signatures
- Enumerations
- Static factory methods
  - Not in SIDL
- Basically the SIDL

Cool Things

- Multiple import roots
  - Necessary for componentized development
- Function pointers (closures)
  - Dispatch from a suitable C wrapper
  - Alternative to interfaces (SIDL)
  - Type checking is dynamic (an exception thrown on arg mismatch)

Multiple Import Roots

- Hooks Modifications
  - Augment the default search path
- Loader Modifications
  - **find_module()** now returns a list of paths
- Importer Modifications
  - Module **__path__** member is now a list
  - Install custom loader and importer
- Installation

```
loader   = Loader(Hooks())
importer = Importer(loader)
importer.install()
```

- Code in `$PETSC_DIR/python/sidl/BuildSystem/importer.py`

Function Pointers

- Input is parsed as a object pointer in the C API
- A C dispatch function is set as the callback
  - The object pointer becomes the context arg
- The dispatch function calls the method with appropriate args
  - Of course, no context arg (come from lexical scope)

Distributing the Wrappers

- All implementations distribute
  - C that links to the Python library and PETSc
  - Some Python
- SIDL version is currently in PETSc
  - Configure with `-with_python -with_shared -with_dynamic`
  - Other versions will be released this fall (distutils)
- Harder to distribute construction mechanism

Examples

- 2D Poisson
  - Finite Differences
  - `$PETSC_DIR/src/snes/examples/tutorials/ex1.py`
- 2D Bratu
  - $-\Delta u - \lambda e^u = 0$
  - Finite Differences
  - `$PETSC_DIR/src/snes/examples/tutorials/ex2.py`
- 2D Poisson
  - P_1 finite elements
  - `petsc4py/test/test_poisson2.py`

The Future

What I Would Do Differently

- Allow Python to handle:
  - Object structure
  - Dynamic loading
- Automate double dispatch
  - Could allow mixing precisions
- Better semantics
  - Specify who is responsible for memory

Shameless Plugs

FENICS Project:

http://www.fenics.org

- FInite element Automatic Tabulator
  - Declarative specification of elements
  - Library of quadratures and shapes
  - Generates complete discrete jet of an element
- Fenics Form Compiler
  - Constructs element tensors from weak forms
  - Generates source code
  - Uses FIAT and exact quadrature