PyTRT: a Python/C++ framework for transport methods development

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PyTRT

MICHIGAN

NEUP Nuclear Energy University Programs

U.S. Department of Energy

Outline

1. Introduction
2. Object-oriented boundary conditions
3. Python
4. Conclusions

Design goals

Primary mission

To graduate in a timely manner.

- rapid, error-free implementation of new methods,
- easy definition of multiple-method test problems,
- high-performance solver kernels to run the problems quickly,
- powerful data analysis tools driven by user needs (me), and
- automated generation of high-quality figures.

Capabilities

Cartesian product of methods:

- Steady-state, linear time-dependent, and nonlinear (semi-implicit) TRT
- 1-D, Flatland, 2-D
- Monte Carlo, S_N transport, diffusion, P_1, anisotropic diffusion

Analysis:

- Lineout
- Angleout
- Matrixout
- Silo for VisIT

Techniques

Reliability:

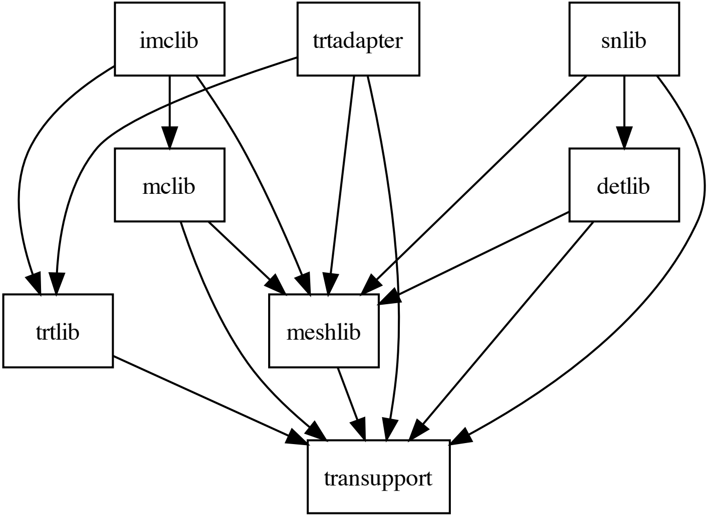
- CMake build process
- Git for version control
- Unit tests (regression)
- Design By Contract
- Modular design
- Trilinos for linear algebra*

Code reuse:

- Template on geometry, etc.
- Python wrapper handles linearization
- Python handles all the stuff that only needs to happen once

*Two-edged sword in terms of reliability

Modular design



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Object oriented boundary conditions

- Abstract `BoundaryCondition` class:
    - At least one `apply` method
    - Other methods like `getIncidentSourceRate`
- Generic `BcManager` class:
    - The problem definition contains a `BcManager` object
    - Vector that maps `BoundaryFace` to `BoundaryCondition*`
    - Functors to help with modifying multiple boundary conditions

Diffusion/constructed matrix

```
void MyBc::apply(const BoundaryFaceT& bface,
                 ProxyVector& vec) const
{
    const CellT& cell = *insideBoundaryCell(&bface);
    source.getFlux()[ cell ] += /* some value */;
}

void apply(const BoundaryFaceT& bface,
           Operator& matrix) const
{
    const CellT& cell = *insideBoundaryCell(&bface);
    matrix.startRow( matrix.getFlux()[cell] );
    matrix.pushRowElement( matrix.getFlux()[cell], /*val*/);
    matrix.finishRow();
}
```

Diffusion/constructed matrix

Called after initializing source vector:

```
bcs.apply( <Traits::BcManagerT, ProxyVector>(sourceVec) );
```

Called after the internal part of the diffusion matrix has been built:

```
startMatrix( ACCUMULATE );
bcs.apply(BcOperatorApplier<Traits>(*this));
finishMatrix();
```

S_N boundary conditions

```
void ReflectingBoundaryCondition::apply(
        const BoundaryFaceT& bface,
        Vector& source ) const
{
    bool onNegBoundary = bface.getFace()->onNegBoundary();
    unsigned int axis = bface.getFace()->getAxis();
    FluxDiscreteT& sourceFlux = source.getBoundaryFlux()[ bfac
    for (QuadratureSetT::const_iterator angle = qs_.begin();
            angle != qs_.end(); ++angle)
    {
        if (isPositive(angle->getOmega()[axis]) == onNegBounda
            sourceFlux[ *angle ]
                = sourceFlux[ qs_.getReflectedAngle(*angle, ax
        }
    }
}
```

MC boundary conditions

```
template<class ProblemTraits_T>
void VacuumBoundaryCondition<ProblemTraits_T>::apply(
        const BoundaryFaceT& bface,
        ParticleT& particle,
        Tally& tally) const
{
    tally.particleExited( bface, particle );
    particle.markDestroyed();
}
```

Outline

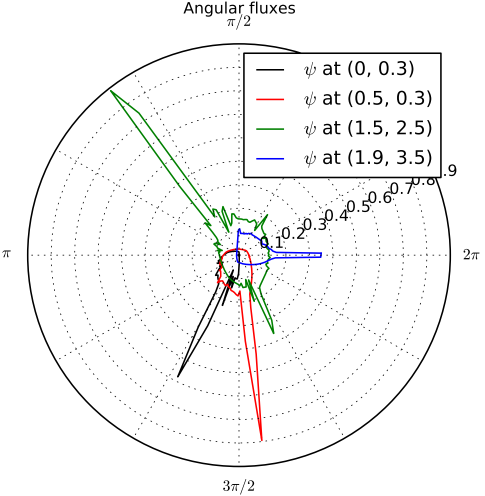
Python structure

- `Manager` class emits C++ problem depending on module passed to it (duck typing)
- `Solver` handles time stepping, callbacks, user feedback, etc.
- Callbacks include Silo output, liveplot, lineout, angleout, MC particle tally info, Δt vs. t, etc.
- Lineout etc. use PyTables to store HDF5 data and metadata

High-level "glue" written in Python:

- Flux-limited diffusion
- Linearization scheme
- Multigrid management
- Time-dependent "events"

Angleout


Angular fluxes
$\pi/2$
π
2π
$3\pi/2$
0.1
0.2
0.3
0.4
0.5
0.6
0.7
ψ at (0, 0.3)
ψ at (0.5, 0.3)
ψ at (1.5, 2.5)
ψ at (1.9, 3.5)

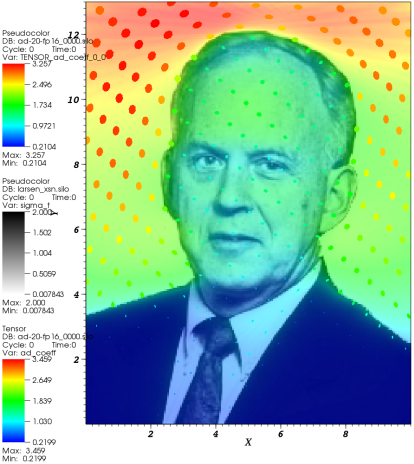
Outline

Availability

Sponsored by the public, available to the public. (Simplified BSD license.)

pytrt.org

Questions?



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