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Title: Recent and Future MCNP6 Capabilities for Radiation Effects / Hostile Environments (U)

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Recent and Future MCNP6 Capabilities for Radiation Effects / Hostile Environments

ABSTRACT

This presentation provides an overview of some recent and future MCNP6 capabilities that may be useful for radiation effects / hostile environment studies.

Outline

- **Nested DXTRAN**
  - complete in MCNP6 trunk
- **Variable Density (for atmospheric studies)**
  - currently being implemented and tested in MCNP6
- **Deterministic adjoint generated weight windows**
  - some work already completed in MCNP6
  - some funding for additional work in FY10
  - work to do beyond FY10

Nested DXTRAN

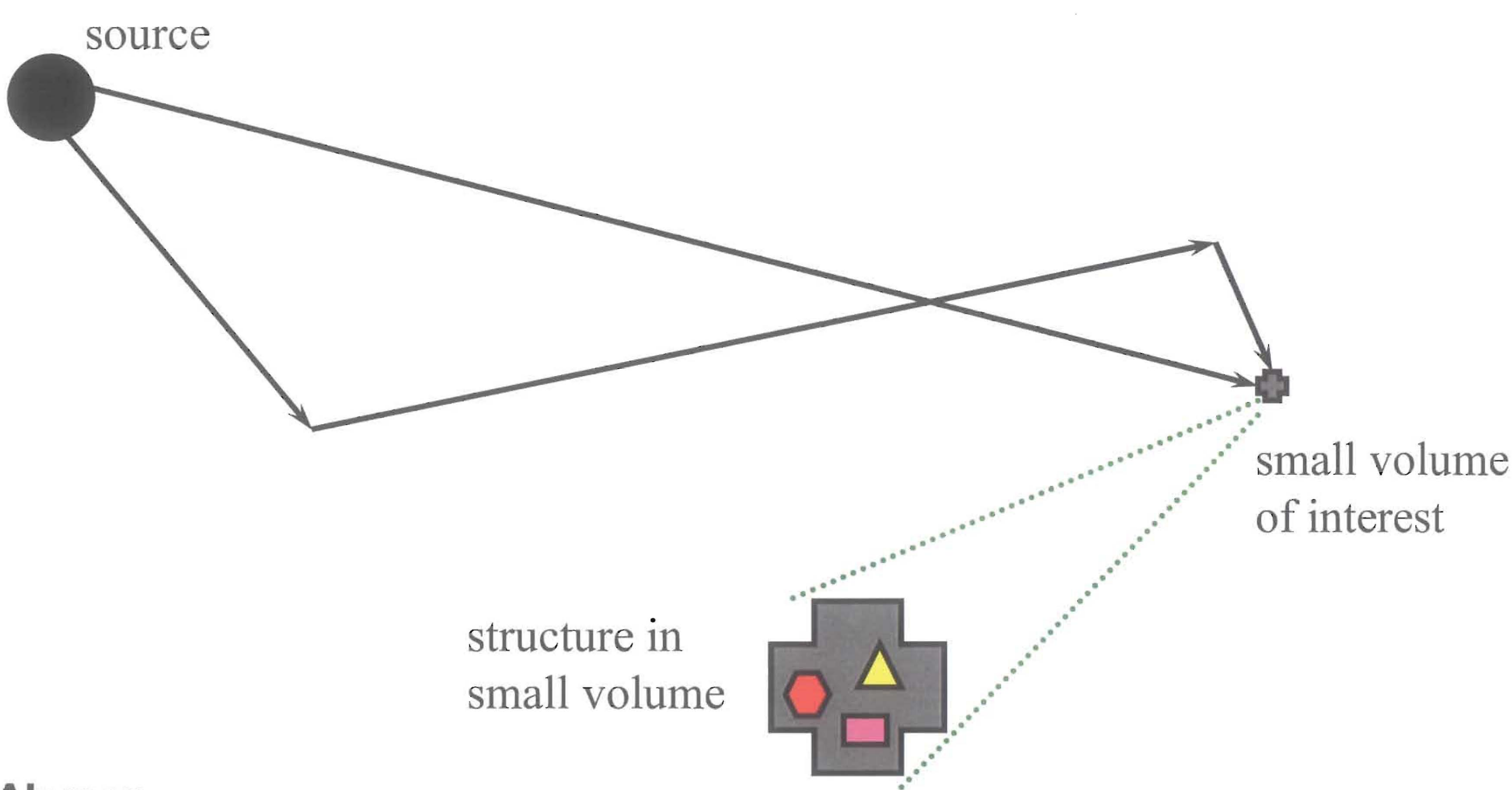
A Variance Reduction Technique

Motivation

- Current DXTRAN technique has problems in scattering media.
- Nested DXTRAN spheres (combined with weight windows) ensures appropriate weights in and about the tally region.
- Helps solve many extremely angle-dependent problems such as computing fluxes in small bodies located in the atmosphere.

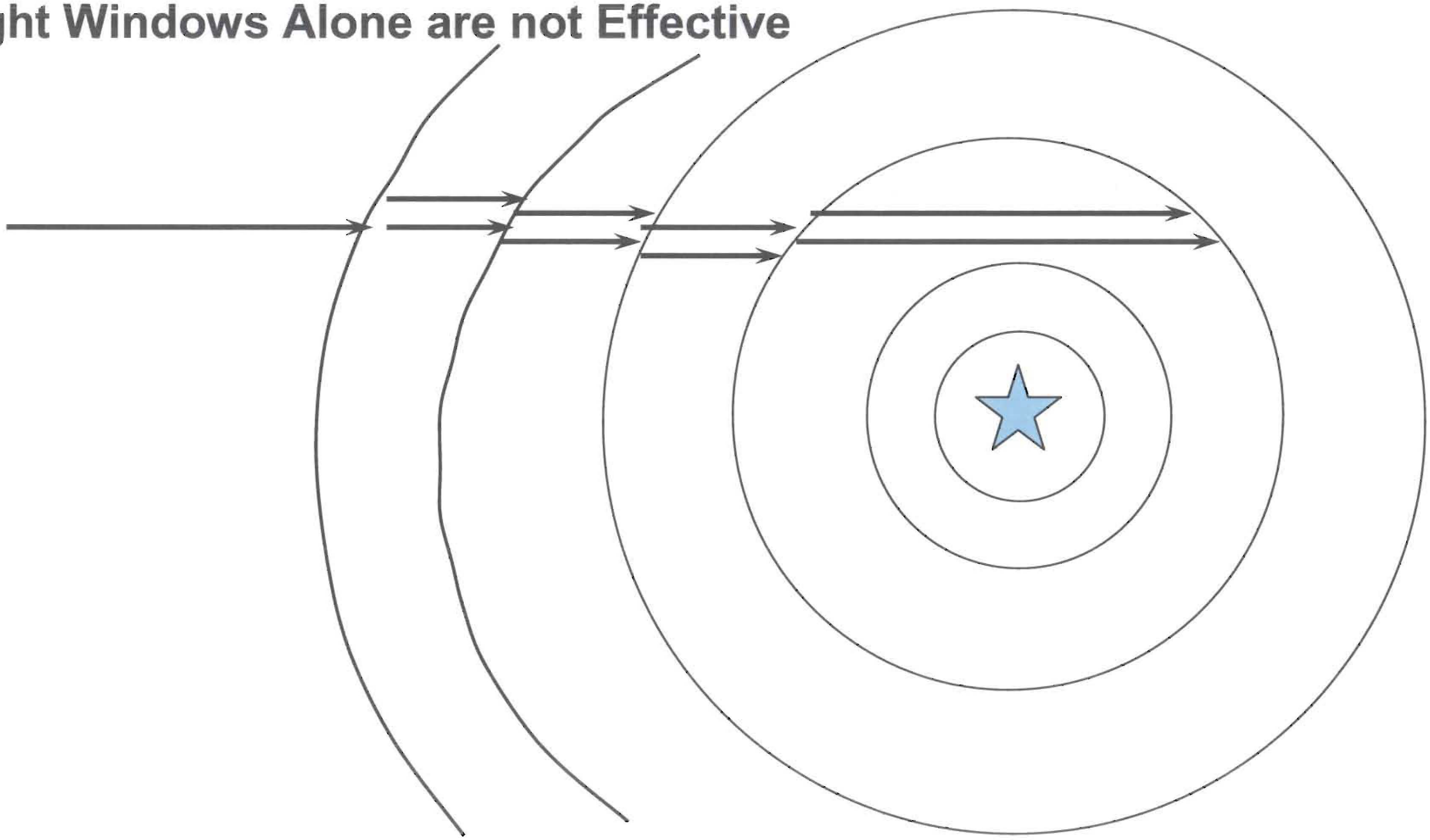
Nested DXTRAN

- **Particle random walks are very unlikely to get to a small volume**



Nested DXTRAN

Weight Windows Alone are not Effective



Splitting does not solve the angle problem

Analog vs Biased Densities / Weighting

DXTRAN partitions the random walk into two parts:

1. Non-DXTRAN particle needs no weight correction - sampled same as w/o DXTRAN.
2. The DXTRAN particle needs a weight correction because it is sampled from a biased density.

true exit angle pdf

$$w_{dxtran} = w\frac{p(\Omega)}{b(\Omega)}e^{-S(\Omega)}$$

biased DXTRAN exit angle pdf

$$b(\Omega) = \frac{1}{\int_{\Omega\_sphere} d\Omega}$$

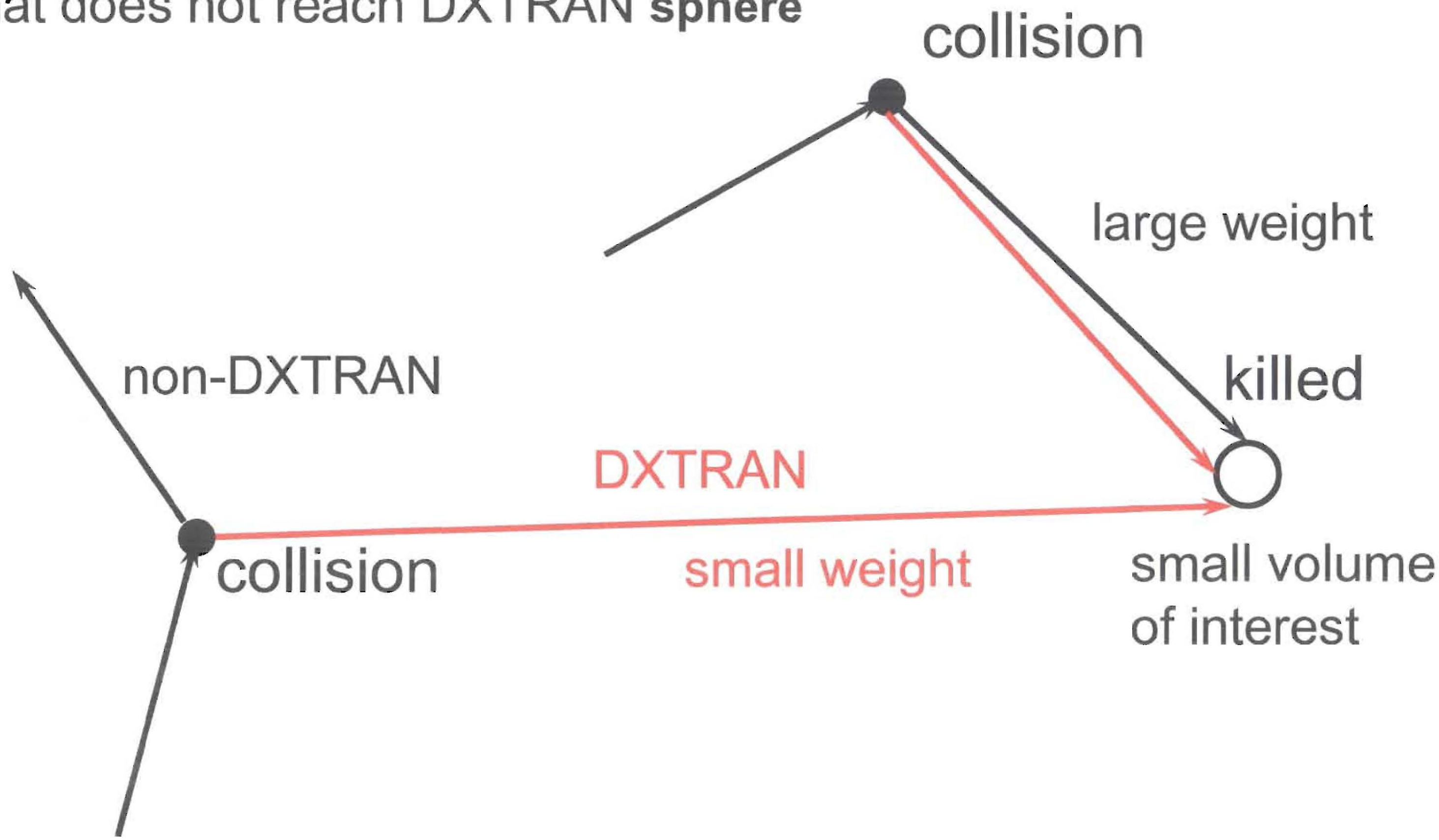
The integration is over all directions pointed toward the DXTRAN sphere from the source or collision exit point.

A fair game because the expected weight is preserved.

Current DXTRAN is a Partial Solution

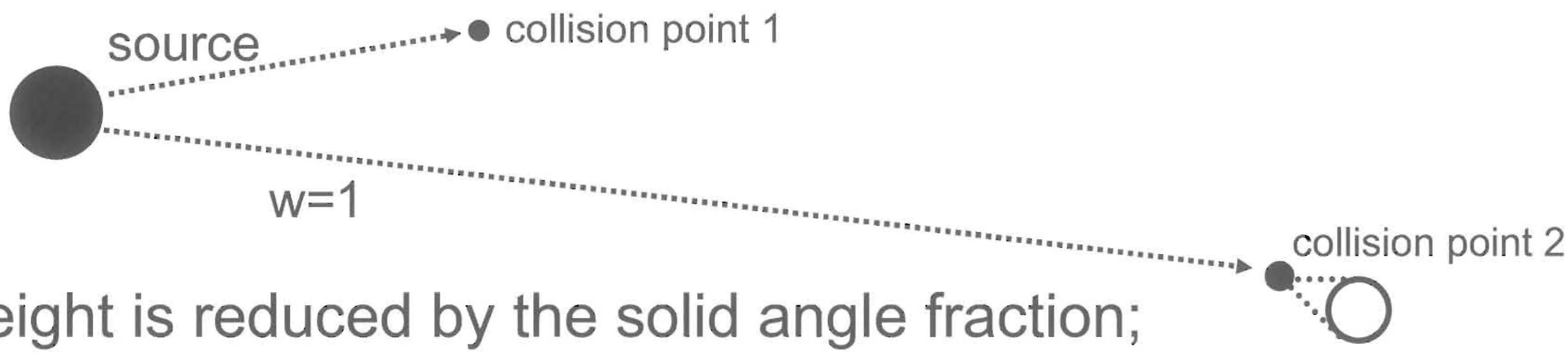
Split particle upon exiting collision:

1. weight that reaches DXTRAN sphere
2. weight that does not reach DXTRAN **sphere**



Current DXTRAN is *Only* a Partial Solution

It is still possible to get large weights in the tally region.



Weight is reduced by the solid angle fraction; there is not much reduction if the collision is close to the sphere.

$$w_{dxtran} = w \frac{p(\Omega)}{b(\Omega)} e^{-S(\Omega)} \qquad b(\Omega) = \frac{1}{\int_{\Omega\_sphere} d\Omega}$$

Note that b will be very large for point 1 but can be as small as $b(\Omega) = \frac{1}{2\pi}$ for point 2 near the sphere surface.

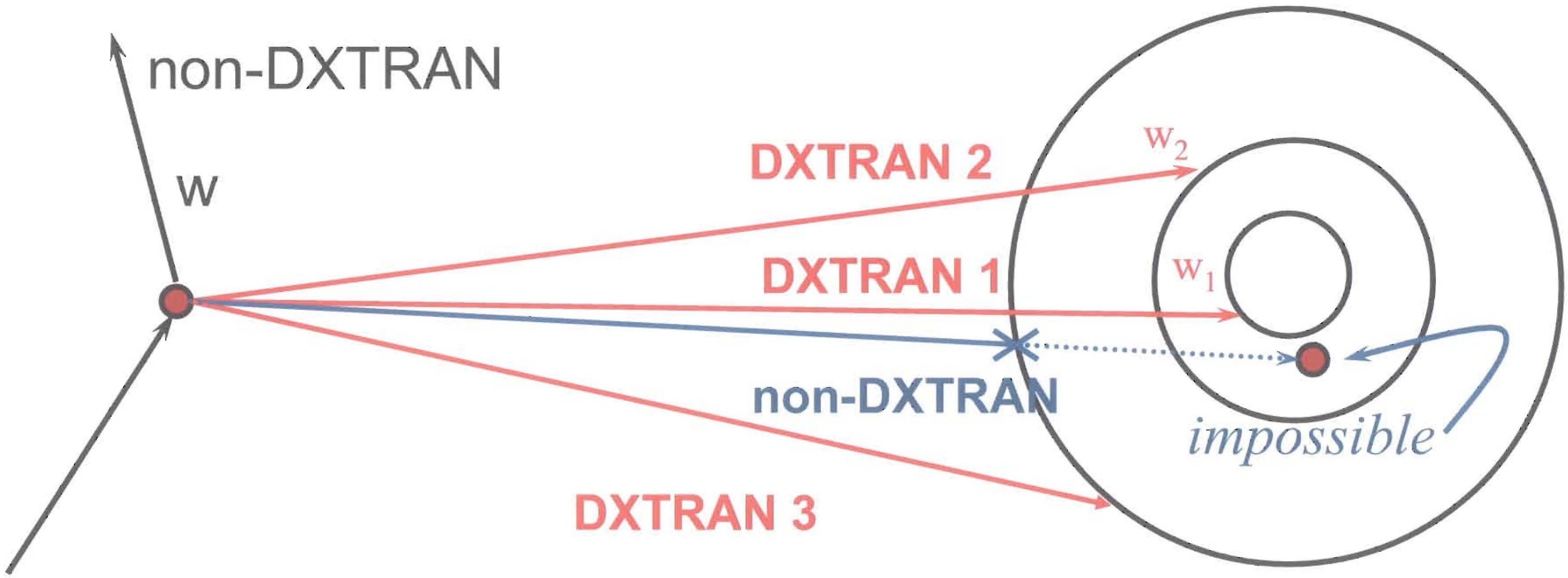
Nesting Precludes Large Weights

- **The first (inner) DXTRAN sphere prohibits a full weight particle from entering the first sphere, but the full weight particle might still collide just before the first sphere (point 2).**
- **A second (outer) DXTRAN sphere surrounding the first ensures that the particle colliding at point 2 cannot have full weight because its weight was reduced by the DXTRAN biasing to the second sphere.**

$$w_{dxtran} = w \frac{p(\Omega)}{b(\Omega)} e^{-S(\Omega)}$$

Nesting Solves Weight Fluctuations

- Sphere n shields all spheres k < n from large weights.
- Continue nesting DXTRAN spheres until the weight window by itself can get enough particles into the vicinity of the outermost DXTRAN sphere with appropriate weight.



Variable Density

Model Improvement

Motivation

- Improve overall accuracy in atmospheric radiation transport problems.
- Generalize variable density treatment for other potential applications.

Variable Density Approaches

- **sub-stepping**

  X-5 Monte Carlo Team, MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, LA-UR-03-1987, Los Alamos, 2003.

- **delta-tracking, hole-tracking, self-scattering, pseudo-scattering, Woodcock tracking**

  E. R. Woodcock et al., Proc. CACMRP65, ANL-7050, ANL, 1965;
  C. J. Everett, E. D. Cashwell, and R. G. Schrandt, LA-5089-MS, US-34, 1972;
  L. L. Carter, E. D. Cashwell, and W. M. Taylor, Nucl. Sci. Eng. 48 (1972) 40;
  S. N. Cramer, ORNL Report ORNL/TM-48880, Oak Ridge, 1977.

- **direct method**

  F. B. Brown and W. R. Martin, Proc. NMCS03, LA-UR-02-6530, 2002;
  F. B. Brown and W. R. Martin, Proc. NECDC 2002, LA-UR-02-6567, 2002;
  F. Brown, D. Griesheimer, W. Martin, Proc. PHYSOR-2004, LA-UR-04-0732.

- **mass integral scaling**

The Chosen Approach: Mass Integral Scaling

In an infinite homogeneous medium with an isotropic point source, the $4\pi R^2$ fluence (time integrated flux) or dose is a function only of ρR, the mass per unit area between the source and receiver, known as "mass range" or "areal density".

Mathematically, the mass scaling law can be derived:

A) using the Boltzmann transport equation:

C. D. Zerby, "Radiation Flux Transformation as a Function of Density in an Infinite Medium with Anisotropic Point Sources," ORNL Report 2100, Oak Ridge, 1965.

B) from the diffusion equation:

Raymond A. Shulstad, "An Evaluation of Mass Integral Scaling as Applied to the Atmospheric Radiation Transport Problem," PhD thesis, Air Force Institute if Technology (AFIT/SA), Wright-Patterson AFB, OH, DS/PH/76-3, 1976.

Previous Implementations

Mass Integral Scaling Approach has been widely used to study the transport of radiation in homogeneous media and in atmosphere:

ATR: R. J. Harris, J. H. Lonergan, and L. Huszar, "Models of Radiation Transport in Air – The ATR Code," SAI-71-557-LJ, La Jolla, CA, Science Applications, Inc., May 1972.

CDR: J. E. Campbell, S. A. Dupree, and M. L. Forsma, "CDR: A Program to Calculate Constant Dose Range from a Point Source of Radiation in the Atmosphere," NWEF 1081, Kirtland AFB, NM: Naval Weapons Effects Facility, 1971.

SMAUG: Harry M. Murthy, "A User Guide to the SMAUG Computer Code," AFWL-TR-72-3, Air Force Weapon Laboratory, Kirtland AFB, NM, May 1972; "A User Guide to the SMAUG-II Computer Code," Air Force Weapon Laboratory, Kirtland AFB, NM, 4 March 1981.

MCNP3B: David L. Monti, "High Altitude Neutral Particle Transport Using the Monte Carlo Simulation Code MCNP with Variable Density Atmosphere," Thesis, Air Force Institute of Technology, AFIT/GNE/ENP/91M-6, Wright-Patterson Air Force Base, Ohio, March 1991; "Modifications to MCNP, Version 3B: Incorporating a Variable Density Atmosphere," Air Force Institute of Technology Technical Report: AFIT/EN-TR-91-2, Wright-Patterson AFB, OH, March 1991.

Mass Integral Scaling Approach

If identical isotropic point sources are placed in two infinite homogeneous air media (medium A and medium B), and if two slant ranges, R_A and R_B, in the two media are related by

$$\rho_A R_A = \rho_B R_B \,, \qquad (1)$$

where ρ is the density in the respective media, then:

$$4\pi R^2_A F(R_A, E) = 4\pi R^2_B F(R_B, E) \,. \qquad (2)$$

If medium B is real air (not homogeneous at all) described by the U. S. Standard Atmosphere, then its "mass range" is defined as $\int \rho_B(Z) dR_B$ and Eq. (1) can be written as:

$$\rho_A R_A = \int \rho_B(Z) dR_B \qquad (3)$$

Deterministic Adjoint Weight Window Generator

(DAWWG)

A Variance Reduction Technique

Motivation

- Research (Wagner, et. al., Larsen, et. al.) have shown that deterministic methods have been effective in generating weight window lower bounds. The methodology is mature.
- These method(s) can be automated, saving user set up time.
- Less user experience with tuning variance reduction techniques is required.

Overview

- The MCNP geometry is "converted" to a mesh representation.
  - Combinatorial geometry is "sampled" based on the weight window mesh.
  - Unstructured mesh can be either "sampled" or used directly.
- A computationally cheap adjoint problem is solved using an S_n deterministic particle transport or diffusion code.
  - Deterministic solution only needs to be "good enough".
- The weight window lower bounds are calculated from the adjoint flux.
- Source biasing is set so that particles are produced with weights within the weight windows.

Chronology For MCNP

- **Circa 2005: Jeremy Sweezy's initial implementation.**
  - script driven
  - PARTISN deterministic solver used in stand alone mode.
- **Summer 2009: Travis Trahan (summer student) resurrects pervious work and starts move away from scripts.**
- **Summer 2009: funding secured for FY10 to upgrade standalone Capsaicin (S_n, unstructured mesh) for 3-D neutronics & adjoint capability, add collision importance to PARTISN, replace AVATAR capability in PARTISN with one that relies on binary files.**
- **Beyond FY 2010: finish linking to deterministic codes & implementing methodology in MCNP, testing, documentation, publication.**

Concerns

- Multi-group cross sections are "limited".
  - Funding needed to "produce" more cross section sets in NDI format
- Work may be needed to "fix up" unstructured mesh geometries for deterministic code use or to make deterministic solvers more forgiving with gaps and overlaps.
- Others?