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CADIS and FW-CADIS

Making an Importance/Weight Map

How do we assign importances to a problem? We can do it by hand. E.g. you can assign each geometry component an importance based on what you think should be happening. All splitting and rouletting is based on the importance ratios between geometric cells. Guidance to do this is to keep adjacent cells within a factor of a few of one another and to keep cells only about two mean free paths thick. It is one thing to think about doing that in a 1D slab (and it still may be too hard to do—think about doing that accurately for a six-order-of-magnitude fall off over 30 cm of lead), but choosing these properly in 3D? Not so easy...

We would prefer to have an automated method that does not rely on guessing. The Consistent Adjoint Driven Importance Sampling (CADIS) and Forward Weighted (FW)-CADIS methods do just that. They were developed by John Wagner, Ali Haghighat, and Douglas Peplow at Penn State and ORNL. We'll go through these methods, highlighting conceptual ideas. In particular, we note the application of the adjoint.

The forward flux describes the particle distribution as a result of system conditions.
The *adjoint* flux describes how important the particle distribution is to the answer in question:

$$-\hat{\Omega}\cdot\nabla\psi^{\dagger}(\vec{r},E,\hat{\Omega})+\Sigma_t(\vec{r},E)\psi^{\dagger}(\vec{r},E,\hat{\Omega})=$$
$$\int_0^{\infty}\int_{4\pi}\Sigma_s(\vec{r},E\rightarrow E',\hat{\Omega}\rightarrow\hat{\Omega}')\psi^{\dagger}(\vec{r},E',\hat{\Omega}')d\hat{\Omega}'dE'+Q^{\dagger}(\vec{r},E,\hat{\Omega}).$$

Note the differences – the streaming term is negative on the left hand side of the equation and the scattering term has particles going "backwards" in energy and angle. We can think of this as asking: how did the particles get from where they started to our response of interest?

The solution to the adjoint equation can be interpreted physically as particle importance. If the adjoint flux in a region is high, then particles there are likely to contribute to our forward response of interest, and we can say that that region is important. On the other hand, if the adjoint flux is low in a given region, it is unlikely that particles in that region will reach the detector in the forward problem, so we can say that that phase space region is less important.

Consider the plots in Figure 1 below.

The left plot is the "forward solution"; particles start at the source and we're interested in the

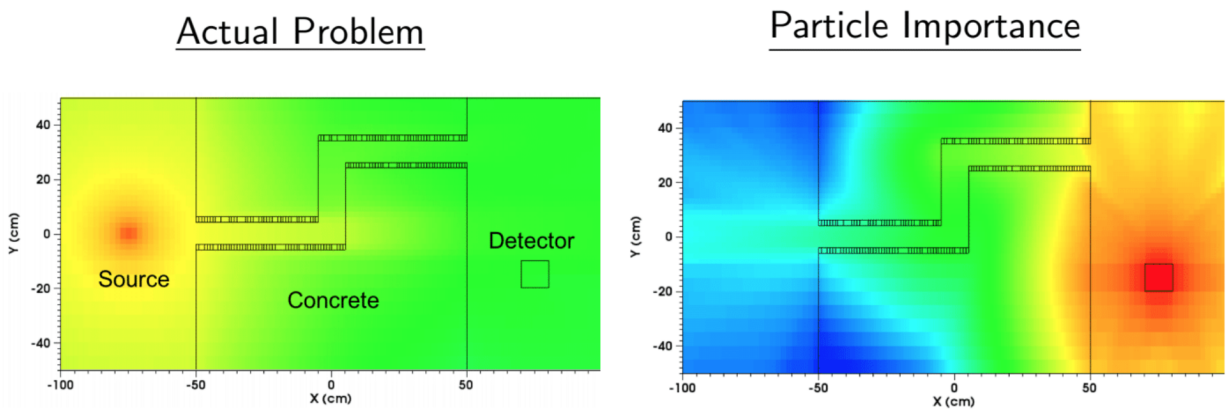

Figure 1: Forward and adjoint scalar flux solution plots.

response at the detector. The right plot is the "adjoint solution"; we set the adjoint source to be the detector and then interpret the resultant adjoint scalar flux solution as our importance map. So, looking at the plot, we see that the bottom left corner of the concrete shield is not a very important region of our phase space; it's unlikely that a particle there will ever reach the detector in the forward problem.

It can be shown that some response of interest R can be calculated as

$$\begin{aligned} R &= \int dV \int dE\, f(\vec{r}, E)\phi(\vec{r}, E) \quad \text{and} \\ &= \int dV \int dE\, \phi^{\dagger}(\vec{r}, E)q(\vec{r}, E) \end{aligned}$$

where f is the response function of interest and angle is neglected for simplicity. This is done by setting $Q^{\dagger} = f$ and using the adjoint identity.

The physical interpretation of the adjoint flux is the influence or importance of a particle in phase space to what we used for the adjoint source: it maps source particles directly into the response. Thus, if we set the response that we are solving for to be the adjoint source, the adjoint flux is the importance map corresponding to that response.

CADIS

These notes are derived from the SCALE manual descriptions.

Note that if we had an accurate representation of $\phi^{\dagger}$, we would then just have the answer. Solving for $\phi^{\dagger}$ is just as hard as solving for ϕ. The idea motivating CADIS is to use an approximate version of $\phi^{\dagger}$ that was obtained quickly with a deterministic solver to create VR parameters for MC.

We use the adjoint flux to bias the source distribution, set target weights, and choose particle birth weights:

$$\hat{Q}(\vec{r}, E) = \frac{1}{R} Q(\vec{r}, E)\phi^{\dagger}(\vec{r}, E)$$
$$w_{nom} = \frac{R}{\phi^{\dagger}(\vec{r}, E)}$$
$$w_0 \equiv \frac{Q(\vec{r}, E)}{\hat{Q}(\vec{r}, E)} = \frac{R}{\phi^{\dagger}(\vec{r}, E)} ,$$

where w_0 is birth weight. Note that we need to set the birth weight this way such that a fair game is preserved given the biased source sampling.

Further, notice that the birth weight exactly matches the target weight. This means that computational time is not wasted splitting/rouletting particles immediately upon birth. The *consistency* among these items is also the source of the method's name.

Multiple Tallies

What if we want multiple tallies? For these problems, the user must accept a total simulation time that is controlled by the tally with the slowest convergence and simulation results where the tallies have a wide range of relative uncertainties.

The obvious way around this problem is to create a separate problem for each tally and use CADIS to optimize each. Each simulation can then be run until the tally reaches the level of acceptable uncertainty. For more than a few tallies, this approach becomes complicated and time-consuming for the user. For mesh tallies, this approach is not reasonable.

Another approach to treat several tallies, if they are in close proximity to each other, or a mesh tally covering a small portion of the physical problem, is to use the CADIS methodology with the adjoint source near the middle of the tallies to be optimized. Since particles in the forward Monte Carlo simulation are optimized to reach the location of the adjoint source, all the tallies surrounding that adjoint source should converge quickly.

The drawback to this approach is the difficult question of "how close". If the tallies are too far apart, certain energies or regions that are needed for one tally may be of low importance for getting particles to the central adjoint source. This may under-predict the flux or dose at some of the tally sites.

For several tallies that are far from each other, multiple adjoint sources could be used. In the forward Monte Carlo, particles would be drawn to one of those adjoint sources. The difficulty with this approach is that typically the tally that is closest to the true physical source will converge

faster than the other tallies. Finding the correct relative source strengths so that all of the tallies converged to the same relative uncertainty in one simulation then becomes an iterative process for the user.

FW-CADIS

If we want the answer everywhere or in many locations (like in shielding or some reactor and security calculations), we need a different approach: forward weighting. There are two ways to think about why this works:

1. In order to converge several tallies to the same relative uncertainty in the one simulation, the adjoint source corresponding to each of those tallies needs to be weighted inversely by the expected tally value.

With mesh tallies, instead of using a uniform adjoint source strength over the entire mesh tally volume, each voxel of the adjoint source should be weighted inversely by the expected forward tally value for that voxel. Areas of low flux or low dose rate would have more adjoint source strength than areas of high flux or high dose rate.

First, a forward, coarse deterministic calculation is done to estimate the expected tally results. A total adjoint source is constructed, where the adjoint source corresponding to each tally is weighted inversely by those forward tally estimates.

2. (from Wagner) To get uniformly-low statistical uncertainty, it has been proposed that the distribution of MC particles should be uniform throughout the system. Although this is not a 'physical' response, it does intuitively represent a desirable objective for obtaining uniform uncertainty. Using adjoint transport theory, we can define the adjoint source such that the result is an importance function targeting uniform particle distribution.

Either way you want to think about it, we do the same thing. We do a coarse deterministic calculation to get the forward flux and use it in constructing the adjoint source:

$$\text{Energy- and space-dependent flux, } \phi(\vec{r},E): \quad Q^{\dagger}(\vec{r},E) = \frac{1}{\phi(\vec{r},E)}$$

$$\text{Space-dependent total flux, } \int dE\ \phi(\vec{r},E): \quad Q^{\dagger}(\vec{r},E) = \frac{1}{\int dE\ \phi(\vec{r},E)}$$

$$\text{Space-dependent total dose rate, } \int dE\ \phi(\vec{r},E)\Sigma_d(\vec{r},E): \quad Q^{\dagger}(\vec{r},E) = \frac{\Sigma_d(\vec{r},E)}{\int dE\ \phi(\vec{r},E)\Sigma_d(\vec{r},E)}$$

You can see the inverse weighting discussed in explanation (1), or you can think of how this impacts

the approximate response (in this case defined as $\langle \phi, Q^{\dagger} \rangle$) for explanation (2):

$$R(\vec{r}, E) = \int dV \int dE \, \phi(\vec{r}, E) \frac{1}{\phi(\vec{r}, E)} \approx 1 \, ,$$

where the approximately equals is because the ϕ values are rough guesses and can come from different calculations.

Again, if we had the global solution, wouldn't we be finished? The key to FW-CADIS is to remember that both the forward and adjoint calculations are coarse and hence very fast. It therefore takes a small amount of time to create a very effective set of values used for source biasing, birth weight setting, and weight window creation - where the weight windows are used for splitting and rouletting.