Draft document

Summer Project on Exponential Convergence For IMC

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1. Introduction

I want to look at modifying the Morel and Bolding [1] algorithm in two ways. One is to remove the need to represent the intensity in a deterministic form and for a deterministic representation of a transport operator. The second is to look at representing the moments of the source with a simpler form that doesn't require as many terms.

Morel and Bolding also didn't include scattering in their formulation. IMC has a lot of scattering occurring because of the effective scatters. I think that scattering can be added to the method, but I think that will require more than a summer's worth of work. So we'll just ignore scattering, and just look at problems with a huge c_v so that there is no effective scattering.

2. Brief ECMC description

Let's say we want to solve

$$\mathcal{T}(I) = S \,, \tag{1}$$

where $\mathcal{T}$ is a linear Monte Carlo operator, I is the unknown, and S is the source. If we could solve Eq.(1) exactly, we'd be done. But let's say we can only approximately solve Eq.(1) with an approximate source S_0 for an estimate of the answer, I_0. Then we can improve I_0 by solving for a correction I_1. We want to solve

$$\mathcal{T}(I_0 + I_1) = S \,, \tag{2}$$

and we can use the linearity of $\mathcal{T}$ to get an equation for the correction I_1:

$$\mathcal{T}(I_1) = S - \mathcal{T}(I_0) = S - S_0 \,. \tag{3}$$

If we don't think $I_0 + I_1$ is accurate enough, we can keep iterating until the source $S - S_0$ is small (in some sense).

We can apply this to a Monte Carlo solution of Eq.(1). In that case, the source S is approximated by a sum of delta functions, because we are sampling discrete particle positions. So we get our approximate solution I_0 by solving

$$\mathcal{T}_{MC}(I_0) = S_{MC} = \Sigma_p s_p \delta(x - x_P) \,, \tag{4}$$

and then the equation for the correction I_1 looks like this:

$$\mathcal{T}_{MC}(I_1) = S - \mathcal{T}(I_0) = S - S_{MC} = S - \Sigma s_p \delta(x - x_P) \,. \tag{5}$$

In solving this equation for the correction, we need to sample Monte Carlo particles from the source term $S - \mathcal{T}(I_0)$. However, we can't do that by sampling from $S - S_{MC} = S - \Sigma s_p \delta(x - x_P)$. This source term has a physical interpretation, but it's not a useful one. The negative delta functions mean "send out negative particles to cancel out the Monte Carlo solution", and S means "Get the answer from the original analytic source like you should have done in the first place". But we can't get the analytic answer from S, or we would have done it already.

ECMC solves the problem of sampling from the source $S - \mathcal{T}(I_0)$ by replacing the operator $\mathcal{T}$ in the source term with a deterministic approximation, which is applied to some smoothed version of the Monte Carlo solution of I_0:

$$\mathcal{T}_{MC}(I_1) = S - \mathcal{T}_D(\{I_0\}) \; . \tag{6}$$

Here $\{\}$ represents some smoothing operator, like representing I_0 with some kind of low-order basis functions. The source in Eq.(6), $S - \mathcal{T}_D(\{I_0\})$ is a continuous function in each zone (or at least it doesn't have delta functions in it), and it can be used as a PDF that we can sample particle positions from. However, it might be negative for some values of x, so we will end up with negative weight particles.

In ECMC, we keep iterating on Eq.(6) until the source $S - \mathcal{T}_D(I_i)$ is "small". The exact source S is usually a smooth, slowly varying function in each zone; for example, with thermal emission, it's linear in space and evenly distributed over the time step. That means that we can probably make at least a few moments of the source small. That is, we can probably make $S - \mathcal{T}_D(\{I_0 + I_i + ...\})$ small.

There are two things that I want to modify in ECMC. The first is getting rid of the deterministic approximation, and the second is getting rid of the need for multiple transport solves. (Really there are three that I want to modify - I want to get rid of the negative particles, but that's a lot harder and I don't know how to do it.)

The way we can get rid of the deterministic solution is to apply the Monte Carlo version of the operator $\mathcal{T}_{MC}$ to the Monte Carlo solution in Eq.(5). The math for this is in section 3, but the result can be seen in Eq.(5) already. If we have solved $\mathcal{T}_{MC} = S_{MC}$ exactly, with no additional statistical noise, then the source term for I_1, which represented by a set of new Monte Carlo particles, is $S - S_{MC} = S - \Sigma s_p \delta(x - x_P)$. That is, the source for the correction is calculated from the particles we used to represent the source - we don't have to tally them into some deterministic I_D, and then apply a deterministic transport operator $\mathcal{T}_D$ to it. We do have to smooth it, however, since we don't want to interpret the delta functions as negative weight particles that cancel out our earlier Monte Carlo solution. So the source term we will really use is $S - \{S_{MC}\} = S - \{\Sigma s_p \delta(x - x_P)\}$.

This is also the way we can get rid of the multiple transport solves. Since all of the Monte Carlo particles are advanced independently, we don't need to wait until one set is done to create the next set. We sample the source S like we always do, and get a bunch of particles. Before we run them, calculate $S - \{\Sigma s_p \delta(x - x_P)\}$. This means we are going to smooth the delta function source that was represented by the particles, by representing it with some low order basis functions, and subtract that from the physical source. That gives us a new PDF, and we sample more particles from it, and we keep going until $S - \{\Sigma s_p \delta(x - x_P)\}$ is small enough. Then we transport all of the particles - there is no need to run them in batches.

So we are going to solve

$$\mathcal{T}_{MC}(I) = S - \{\Sigma s_p \delta(x - x_P)\} - \{\Sigma s_q \delta(x - x_q)\} - ... \tag{7}$$

where the first N_p particles are drawn from a PDF calculated from the source S, the next N_q are drawn from a PDF calculated from the source $S - \{\Sigma s_p \delta(x - x_P)\}$, etc, until we think the source is small enough.

This becomes more complicated when we do some statistical operation on the particles while we are advancing them. In that case, it isn't true that $\mathcal{T}_{MC} = S_{MC}$ exactly, so the second equality in Eq.(5)

doesn't hold exactly. This happens when we do scattering, for example, where we sample a new random direction for the particle after it is born. In that case, we have to iterate. We would end up running the particles and tallying a source term based on the difference between the PDF for scattering angle and the directions we actually sampled for the scattered particles. But we're going to ignore that situation for now.

So the project involves generating source particles, calculating $S - \{\Sigma s_p \delta(x - x_P)\}$, sampling more source particles, recalculating $S - \Sigma s_p \delta(x - x_P)$, etc, until they are done. Then we run them to the end of the time step, and see how noisy the solution is. The question is how big a reduction in statistical noise we see.

An example for what I mean by $\{\}$ is the standard linear finite element basis functions $B_0 \equiv x$ and $B_1 \equiv 1 - x$. Let's look at an infinite medium problem first. Then the only coordinate that matters for the particles is time. Say we are sampling the source in time in [0,1]. This means we are picking emission times for particles with equal probability in [0,1]. Then we sample a bunch of particles, and then calculate the finite element representation of the source $\Sigma s_p \delta(t - t_P)$:

$$\{\Sigma s_p \delta(t - t_P)\} = c_o B_0(t) + c_1 B_1(t) \tag{8}$$

where the coefficients c_o and c_1 come from doing the standard finite element decomposition to the function $f(t) \equiv \Sigma s_p \delta(t - t_P)$.

When we go to a 1D problem, we have a 3D representation of the source, because we care about t, x, and μ. That means we would have $2^3 = 8$ coefficients for a first order representation, and $(N+1)^3$ coefficients for order N:

$$f(t, x, \mu) = \Sigma_i \Sigma_j \Sigma_k c_{ijk} B_i(t) B_j(x) B_k(\mu) \tag{9}$$

One additional thing I want to look at is whether we can use a reduced basis set for the representation. For example, can we use a separable set of functions. That means replacing Eq.(9) with products of t, x, and μ separately, rather than every possible cross term:

$$f(t, x, \mu) = [\Sigma_i \tau_i B_i(t)][\Sigma_j \chi_j B_j(x)][\Sigma_k \theta_k B_k(\mu)] \tag{10}$$

This would reduce the number of coefficients to $3N$ for order N. (See section 4 for details.)

A lot of code is already written. I have written code that will let us use the Bernstein polynomials of order 1 and 2 as basis functions for the smooth representation of the source. I stuck it into the thermal photon source, and I created particles, calculated the moments, and created more particles until the source was small. I did this for both the standard finite element representation and the separable one. The separable one seems to work, but the standard one doesn't seem to drive the moments to a small value. I'm sure it's a bug, so investigating this and fixing it would be your first task.

3. MC representation of $\mathcal{T}$, I and the source S_{MC}

To eliminate the need for the deterministic I and deterministic transport operator, we apply the Monte Carlo version of the transport operator to the Monte Carlo representation of I. We're going to ignore scattering and frequency dependence for now. The point of this section is to justify using as a source the term $S - \{S_{MC}\} = S - \{\Sigma s_p \delta(x - x_P)\}$ for the transport equation, as I did in Eq.(7).

The transport equation for thermal radiation is given in [2] Eq. 2.17, p. 13 as

$$\frac{1}{c}\frac{\partial I(x,t,\Omega)}{\partial t} + \Omega \cdot \nabla I(x,t,\Omega) = c\sigma_a(T) a T^4 - \sigma_a(T) I(x,t,\Omega)\ , \tag{11}$$

where $I(x,t,\Omega)$ is the radiation intensity, with units of $\text{energy}/(\text{time length}^2\ \text{frequency solid angle})$, c is the speed of light, T is the material temperature, $\sigma_a(T)$ is the macroscopic absorption opacity in inverse length units and $a = \frac{8\pi^5 k^4}{15c^3h^3}$ is the radiation constant.

Eq.(11) comes with initial conditions $I_{ic}(x,t,\Omega)$ defined for all points in the region of interest, and boundary conditions $I_{bc}(x,t,\Omega)$ defined on the boundary of the region of interest for values of Ω that ensure that I_{bc} describes incoming photons.

Eq. (11) is often solved by Monte Carlo methods. These methods advance solutions of Eq. (11) over a time interval $[t_n, t_n + \Delta t]$ that is small enough that we can regard σ_a as fixed at its t_n values.

For notational convenience, we are going to define transport operator $\mathcal{T}(I)$:

$$\mathcal{T}(I) \equiv \frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I + \sigma_a(T) I \ . \tag{12}$$

Note that $\mathcal{T}$ is linear in I. Eq.(12) allows us to write Eq. (11) as

$$\mathcal{T}(I) = c\sigma_a a T^4 \ . \tag{13}$$

Monte Carlo representation of I is as a collection of particles. Particle p moves along one or more segments with speed c with a fixed direction and frequency. We will assume that the opacity σ_a is constant along each path, with value $\sigma_{a,s}$. The segments cover a time $[t_{s0}, t_{s1}]$. The energy of particle p on segment s, $e_{p,s}$, decreases along each segment at a rate proportional to the absorption opacity and the energy. That is, e_p satisfies

$$\frac{\mathrm{d}e_{p,s}}{\mathrm{d}t} = -\sigma_a \ e_{p,s} \ , \tag{14}$$

yielding

$$e_{p,s}(t - t_{s0}) = e_{p,s}(t_{s0}) \ \exp[-\sigma_{a,s}(t - t_{s0})] \ . \tag{15}$$

The direction could change between segments because of scattering events, but we are ignoring that for now.

The intensity I_{MC} represented by the collection of particles in the simulation is a sum over all paths of all particles. We have

$$I_{MC} \equiv \Sigma_p \Sigma_s I_{p,s} \tag{16}$$

where

$$I_{p,s} \equiv c e_p(t_{s0}) \exp[-c\sigma_{a,s}(t - t_{s0})] \delta^3(x - x_{s0} - c\Omega(t - t_{s0})) \delta(\Omega - \Omega_{p,s}) [H(t - t_{s0}) - H(t - t_{s1})]. \tag{17}$$

Here, $\delta(x)$ is the Dirac delta function, and H is the Heaviside step function. $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x > 0$. In addition, H satisfies $\frac{\mathrm{d}H(x-x_0)}{\mathrm{d}x} = \delta(x - x0)$. $\delta^3(x - x_{s0} - c\Omega(t - t_{s0}))$ is shorthand for $\delta(x - x_{s0} - c\Omega_x(t - t_{s0}))\delta(y - y_{s0} - c\Omega_y(t - t_{s0}))\delta(z - z_{s0} - c\Omega_z(t - t_{s0}))$. The term in H enforces the fact that the contribution on the segment s is non-zero only for times in the range $[t_{s0}, t_{s1}]$.

The statistical and algorithmic choices in the implementation of the algorithm show up as choices for the values of particle properties like $e_p(t_{s0})$, $\Omega_{p,s}$, x_{s0}, etc, and in the choices of the beginning and ending path lengths.

Now we want to apply $\mathcal{T}$ to I_{MC} given by Eq.(16) to get the statistical source. This yields

$$\begin{aligned}\frac{1}{c}\frac{\partial I_{p,s}}{\partial t} &+ \Omega\cdot\nabla I_{p,s} + \sigma_a I_{p,s} = e_{p,s}(t_{s0})\exp[-c\sigma_{a,s}(t-t_{s0})]\delta^3(x-x_{s0}-c\Omega(t-t_{s0})\delta(\Omega-\Omega_{p,s})[\delta(t_{s0})-\delta(t_{s1})] \\ &= e_{p,s}(t_{s0})\delta^3(x-x_{s0})\delta(\Omega-\Omega_{p,s})\delta(t_{s0}) - e_{p,s}(t_{s1})\delta^3(x-x_{s1})\delta(\Omega-\Omega_{p,s})\delta(t_{s1})]\,, \end{aligned} \tag{18}$$

where $e_{p,s}(t_{s1}) \equiv e_{p,s}(t_{s0})\exp[-c\sigma_{a,s}(t_{s1}-t_{s0})]$. The last equality in Eq.(18) holds by virtue of the properties of the δ function - $\delta^3(x-x_{s0}-c\Omega(t-t_{s0})\delta(t_{s0}) = \delta^3(x-x_{s0})\delta(t_{s0})$.

We see that $\mathcal{T}(I_{p,s})$ is the sum of δ functions representing the emission of particles at the beginning of paths, minus the destruction of particles at the end of paths. So then

$$\begin{aligned}\mathcal{T}(I_{MC}) &= \Sigma_p\Sigma_s\mathcal{T}(I_{p,s}) \\ &= \Sigma_p\Sigma_s e_{p,s}(t_{s0})\delta^3(x-x_{s0})\delta(\Omega-\Omega_{p,s})\delta(t_{s0}) \\ &\quad -\Sigma_p\Sigma_s e_{p,s}(t_{s1})\delta^3(x-x_{s1})\delta(\Omega-\Omega_{p,s})\delta(t_{s1})\end{aligned} \tag{19}$$

The sum of the start of the paths is just the source term I said we needed in Eq.(7). The term for the end of the paths would come into play if we were killing particles by Russian roulette, or we were doing scattering. Scattering would be like killing a particle with one value of Ω and creating one with a new value. This is what I meant earlier when I stated that we would have to iterate if we were doing scattering or other statistical changes in particles after they were created. Those changes would show up as a source from particle creation and destruction in Eq.(19).

For now, we are going to ignore scattering and Russian roulette. Then we only have to worry about the source for particle creation. That means that Eq.(7) becomes

$$\begin{aligned}\mathcal{T}_{MC}(I) &= c\sigma_a a T^4(x) \\ &- \Sigma_p e_p(t0)\delta^3(x-x_p)\delta(\Omega-\Omega_p)\delta(t_p) \\ &- \Sigma_q e_q(t0)\delta^3(x-x_q)\delta(\Omega-\Omega_q)\delta(t_q) \\ &\ldots\end{aligned} \tag{20}$$

with $\mathcal{T}_{MC}$ being a Monte Carlo transport solution, and the first N_p particles are drawn from a PDF calculated from the source $c\sigma_a a T^4(x)$, the next N_q are drawn from a PDF calculated from the source $c\sigma_a a T^4(x) - \{\Sigma e_p\delta^3(x-x_p)\delta(\Omega-\Omega_p)\delta(t_p)\}$, etc.

4. Separable basis functions

Look at the case with only one space dimension and time. Approximate the function $f(x,t)$ as a product of a constant and the product of two functions $X(x)$ and $T(t)$:

$$f(x,t) \approx KX(x)T(t), \tag{21}$$

with $X(x)$ satisfying

$$\int_0^1 \mathrm{d}x\; X = 1 \tag{22}$$

and $T(t)$ satisfying

$$\int_0^1 \mathrm{d}t\ T = 1\ . \tag{23}$$

The constant K is defined be requiring that

$$\int_0^1 \mathrm{d}x\ \int_0^1 \mathrm{d}t\ f(x,t) = K\ , \tag{24}$$

which holds if Eqs.(22) and (23) hold.

Now we show how to construct functions $X(x)$ and $T(t)$ which satisfy Eqs.(22) and (23). Assuming for the moment that Eq.(22) holds, we define $T(t)$ via

$$T(t) \equiv \frac{\int_0^1 \mathrm{d}x\ f(x,t)}{K}\ . \tag{25}$$

We expand $T(t)$ in a set of basis functions $B_i(t)$:

$$T(t) = \Sigma_i \tau_i B_i(t)\ . \tag{26}$$

Substituting Eq.(26) into Eq.(25), multiplying by $B_j(t)$, and integrating over time, we get the following linear system

$$\Sigma_i \tau_i \int_0^1 \mathrm{d}t\ B_i(t) B_j(t) = \frac{\int_0^1 \mathrm{d}t\ \int_0^1 \mathrm{d}x\ f(x,t) B_j(t)}{K}\ , \tag{27}$$

which defines the τ_i. Similarly,

$$X(x) = \Sigma_i \chi_i B_i(x) \tag{28}$$

with the χ_i satisfy

$$\Sigma_i \chi_i \int_0^1 \mathrm{d}x\ B_i(x) B_j(x) = \frac{\int_0^1 \mathrm{d}x\ \int_0^1 \mathrm{d}t\ f(x,t) B_j(x)}{K}\ . \tag{29}$$

It remains to show that $X(x)$ and $T(t)$ defined via Eqs.(28) and (26) satisfy Eqs.(22) and (23). We will show that, if the $B_i(t)$ are a partition of unity, then Eqs.(22) and (23) hold. Being a partition of unity means that the B_i satisfy

$$\Sigma_i B_i(t) = 1\ . \tag{30}$$

With $T(t)$ defined by Eq.(26), K defined by Eq.(24), and τ_i defined by Eq.(27), we have

$$\begin{aligned}
\int_0^1 \mathrm{d}t\ T(t) &= \int_0^1 \mathrm{d}t\ \Sigma_i \tau_i B_i(t) \\
&= \Sigma_i \int_0^1 \mathrm{d}t\ B_i(t) \\
&= \Sigma_i \tau_i \int_0^1 \mathrm{d}t B_i(t) \Sigma_j B_j(t) \\
&= \Sigma_j \Sigma_i \tau_i \int_0^1 \mathrm{d}t\ B_i(t) B_j(t) \\
&= \Sigma_j \int_0^1 \mathrm{d}t\ \frac{\int_0^1 \mathrm{d}x\ f(x,t) B_j(t)}{K} \\
&= \frac{\int_0^1 \mathrm{d}t\ \int_0^1 \mathrm{d}x\ f(x,t) \Sigma_j B_j(t)}{K} \\
&= \frac{\int_0^1 \mathrm{d}t\ \int_0^1 \mathrm{d}x\ f(x,t)}{K} = 1.
\end{aligned} \tag{31}$$

A similar computation shows that Eq.(22) is satisfied by $X(x)$ when that function is defined by Eq.(28).

If we have

$$f(x,t) = \Sigma_p e_p \delta(x - x_p)\delta(t - t_p) \ , \tag{32}$$

then

$$\int_0^1 \mathrm{d}t \ f(x,t) = \Sigma_{p\in P(t)} e_p \delta(x - x_p)\delta(t - t_p) \ , \tag{33}$$

where $P(t)$ is the set of all particles with $t_p \in [0,1]$. K satisfies

$$K = \Sigma_{p\in[P(t)\cup P(x)]} e_p \ , \tag{34}$$

the τ_i satisfy

$$\Sigma_i \tau_i \int_0^1 \mathrm{d}t \ B_i(t) B_j(t) = \frac{\Sigma_{p\in[P(t)\cup P(x)]} e_p B_j(t_p)}{K} \ , \tag{35}$$

and the χ_i satisfying

$$\Sigma_i \chi_i \int_0^1 \mathrm{d}x \ B_i(x) B_j(x) = \frac{\Sigma_{p\in[P(t)\cup P(x)]} e_p B_j(x_p)}{K} \ , \tag{36}$$

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References

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