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Validation of a new grid-based Boltzmann equation solver for dose calculation in radiotherapy with photon beams

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Abstract

A new grid-based Boltzmann equation solver, Acuros™, was developed specifically for performing accurate and rapid radiotherapy dose calculations. In this study we benchmarked its performance against Monte Carlo for 6 and 18 MV photon beams in heterogeneous media. Acuros solves the coupled Boltzmann transport equations for neutral and charged particles on a locally adaptive Cartesian grid. The Acuros solver is an optimized rewrite of the general purpose Attila© software, and for comparable accuracy levels, it is roughly an order of magnitude faster than Attila. Comparisons were made between Monte Carlo (EGSnrc) and Acuros for 6 and 18 MV photon beams impinging on a slab phantom comprising tissue, bone and lung materials. To provide an accurate reference solution, Monte Carlo simulations were run to a tight statistical uncertainty ($\sigma \approx 0.1\%$) and fine resolution (1–2 mm). Acuros results were output on a 2 mm cubic voxel grid encompassing the entire phantom. Comparisons were also made for a breast treatment plan on an anthropomorphic phantom. For the slab phantom in regions where the dose exceeded 10% of the maximum dose, agreement between Acuros and Monte Carlo was within 2% of the local dose or 1 mm distance to agreement. For the breast case, agreement was within 2% of local dose or 2 mm distance to agreement in 99.9% of voxels where the dose exceeded 10% of the prescription dose. Elsewhere, in low dose regions, agreement for all cases was within 1% of the maximum dose. Since all Acuros calculations required less than 5 min on a dual-core two-processor workstation, it is efficient enough for routine clinical use. Additionally, since Acuros calculation times are only weakly dependent on the number of beams, Acuros may ideally be suited to arc therapies, where current clinical algorithms may incur long calculation times.

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1. Introduction

The American Association of Physicists in Medicine (AAPM Report 85 2004) recommends that the uncertainty of computed dose distributions should be less than 2%. This accuracy level is generally achievable with modern treatment planning systems in water equivalent phantoms. However, it can be verified only for a limited set of dosimetric tests, normally performed during system commissioning and as a part of a quality assurance program. Owing to the complexity of patient heterogeneities combined with a broad range of external photon beam treatment conditions, larger errors are common in three-dimensional patient dose distributions. A well-documented source of errors is from accuracy limitations in presently employed dose-calculation algorithms (Reynaert et al 2007 and references therein). Current clinical dose-calculation algorithms such as pencil-beam convolution and convolution superposition employ the use of pre-calculated Monte Carlo dose kernels, which are then locally scaled to approximate photon and electron transport in the presence of heterogeneities. Limitations in the accuracy of pencil-beam convolution algorithms in the presence of anatomical heterogeneities have been extensively documented (Knöös et al 1995, Laub et al 2000, Boudreau et al 2005, Krieger and Sauer 2005, Yang et al 2005). While convolution/superposition-based algorithms perform notably better, accuracy may still be compromised in the presence of large density gradients (Arnfield et al 2000, Krieger and Sauer 2005, Paclinck et al 2005, Seco et al 2005), such as those at interfaces between different materials: air, bone, lung and soft tissue. This has lead to a rapidly growing interest in the clinical adoption of Monte Carlo-based dose calculation algorithms (Chetty et al 2007, Reynaert et al 2007). If a sufficiently large number of particle histories are simulated, Monte Carlo will approach the true physical solution within the limits of the particle interaction data and uncertainties in the geometry and composition of the field being modeled. However, a recognized disadvantage of Monte Carlo is long calculation times, especially where statistical noise needs to be minimized and/or a high spatial resolution is required. This has lead to the development of optimized Monte Carlo codes such as Macro Monte Carlo (Neuenschwander and Born 1992), Voxel Monte Carlo (Fippel 1999) and DPM (‘dose planning method’, Sempau et al 2000), to name a few, which through a broad range of acceleration techniques calculate dose fields substantially faster than their general purpose counterparts such as PENELOPE (Bard et al 1995), EGSnrc (Kawrakow and Rogers 2000), MCNPX (Waters 2002) and GEANT (Agostinelli et al 2003). However, due to clinical throughput requirements and the increasing adoption of adaptive image-guided radiotherapies, the dose field may be recalculated prior to each fraction and accurate dose calculation methods such as Monte Carlo remain too slow for effective clinical use.

An alternative to Monte Carlo-based algorithms is methods which directly solve the linear Boltzmann transport equation (LBTE). The LBTE is the governing equation that describes the macroscopic behavior of ionizing particles (neutrons, gamma-rays, electrons, etc) as they travel through and interact with matter. For a given volumetric domain of matter, subject to a radiation source, the solution to the LBTE would give an ‘exact’ description of the dose within the domain. However, since closed form, or analytic, solutions to the LBTE can only be obtained for a few simplified problems, the LBTE must be solved in an open form, or non-analytic, manner. The Monte Carlo method also solves the LBTE, but through random sampling techniques that imitate propagation of radiation in the medium.

Methods which deterministically solve the LBTE can be broadly referred to as grid-based Boltzmann solvers (GBBS), which explicitly solve the LBTE through discretizing in space, angle and energy, and then iteratively solving it (Lewis and Miller 1984). These methods share the common trait of solving the LBTE on a grid of computational elements, and for the
most part, use a similar multi-group treatment in energy. A number of different techniques have been employed to discretize in angle, including discrete-ordinates, spherical harmonics and short and long characteristic methods (Lewis and Miller 1984). As opposed to empirical and correction-based methods as well as pencil-beam and convolution superposition methods, both Monte Carlo and GBBS methods are convergent. That is, with increasing refinement both approaches will converge on the same solution. The achievable accuracy of both approaches is equivalent and is limited only by uncertainties in the particle interaction (cross-section) data and uncertainties in the problem being analyzed. However, in practice, neither Monte Carlo nor explicit LBTE solution methods are exact, and both methods produce errors. In Monte Carlo, errors are stochastic and result from simulating a finite number of particles. When Monte Carlo methods employ acceleration methods such as de-noising or condensed history algorithms, however, systematic errors may also be introduced. In GBBS methods, errors are primarily systematic and result from discretization of the solution variables in space, angle and energy. In both Monte Carlo and GBBS methods, a trade-off exists between speed and accuracy. Reduced computational time may be achieved when less stringent accuracy criteria are specified, and vice versa. The viability of both approaches for clinical treatment planning is therefore based on the achievable combination of calculation speed and accuracy.

While relatively unknown in the radiotherapy community, GBBS methods have been shown to hold potential benefits for dose calculations (Hertel and Murphie 1983, Uwamino et al. 1986, Nigg et al. 1991, Moran et al. 1992, Storr 1992, Gokhale et al. 1994, Nigg and Eng 1994, Daskalov et al. 2000a, 2000b, 2002, Yuan et al. 2008). Due to the complexity of solving the electron transport in three-dimensional space, most research focused on either the application of GBBS methods toward brachytherapy or photon beam radiotherapies using a photon KERMA (kinetic energy released per unit mass) approximation, the latter of which negates the spatial transport of electrons. Recently, the feasibility of GBBS methods for dose calculations using coupled photon–electron transport for MV photon beams was demonstrated (Gifford et al. 2006, Vassiliev et al. 2008) using the general purpose radiation transport software, Attila. Attila is a general purpose GBBS code for which applications range from nuclear fusion (Youssef et al. 2008, Arter and Loughlin 2009) to optical tomography (Rasmussen et al. 2006, Joshi et al. 2008). Attila employs linear discontinuous finite-element spatial differencing on a computational mesh consisting of arbitrary tetrahedral elements. The primary photon fluence is analytically transported through ray tracing, and the discrete ordinates method is used for angular differencing of the scattered fluence. The studies reported that Attila was able to achieve comparable accuracy to Monte Carlo simulations performed to tight statistical uncertainties. As follow-on to Attila, Transpire, Inc. (Gig Harbor, WA) developed a new GBBS solver, Acuros, which was optimized for radiotherapy dose calculations. Acuros represents a ground up rewrite of Attila, with the methods adapted for the specific needs of radiotherapy dose calculations.

In this study we benchmarked the accuracy and speed of Acuros against Monte Carlo for 6 and 18 MV photon beams in heterogeneous media. We used the EGSnrc Monte Carlo code (Kawrakow and Rogers 2000) as it is one of the most comprehensively benchmarked programs in the field. First, we performed a test similar to the ICCR benchmark (Rogers and Mohan 2000, Chetty et al. 2007). The test is considered a standard for code performance evaluation. Dose fields were calculated for square 6 and 18 MV photon beams incident on a 30 cm cubic phantom comprising tissue, bone and lung slabs. For the second test we chose a very common, yet challenging, treatment planning-type calculation. We calculated dose distributions in an anthropomorphic phantom receiving breast irradiation with two tangential fields using a field-in-field technique. The treatment plan was designed following standard treatment planning procedures for breast cancer at M.D. Anderson Cancer Center. This type
of treatment presents computational challenges such as interfaces between different tissues including air, lung, bone and soft tissue. Furthermore, field shapes were defined by a multileaf collimator, and both 6 and 18 MV energies were used.

2. Methods and materials

For a problem spatial domain with volume, V, and surface, δV, Acuros solves the time-independent three-dimensional system of coupled Boltzmann transport equations (LBTE), which are given by (for brevity the dependent variables have been suppressed in the equations)

\[ \hat{\Omega} \cdot \nabla \Phi^{\gamma} + \sigma_{\gamma}^{i} \Phi^{\gamma} = q^{\gamma} + q^{e}, \]  
\[ \hat{\Omega} \cdot \nabla \Phi^{e} + \sigma_{e}^{i} \Phi^{e} - \frac{\partial}{\partial E} (S_{R} \Phi^{e}) = q^{ee} + q^{\gamma e} + q^{\gamma}, \]  

where equations (1a) and (1b) solve for photon, γ, and electron, e, transport, respectively. Here, \( \Phi^{\gamma}(\vec{r}, E, \hat{\Omega}) \) is the photon angular fluence, \( \Phi^{e}(\vec{r}, E, \hat{\Omega}) \) is the electron angular fluence, \( \vec{r} = (x, y, z) \) is the spatial position vector, \( E \) is energy, \( \hat{\Omega} = (\mu, \eta, \xi) \) is the unit direction vector and \( \hat{n} \) is the outward directed unit normal vector to surface \( \delta V \). For equations (1), \( \vec{r} \in V, \hat{\Omega} \in 4\pi \) and \( E > 0 \). Equations (1) are subject to all possible standard boundary conditions on \( \delta V \), the most likely being the vacuum or non-reentrant boundary conditions given by

\[ \Phi^{\gamma} = 0, \quad \text{for} \quad \hat{\Omega} \cdot \hat{n} < 0, \] 
\[ \Phi^{e} = 0, \quad \text{for} \quad \hat{\Omega} \cdot \hat{n} < 0. \] 

The first term on the left-hand side of equations (1) is termed the streaming operator. The second term on the left-hand side of equations (1) is termed the collision or removal operator, where \( \sigma_{\gamma}^{i}(\vec{r}, E) \) and \( \sigma_{e}^{i}(\vec{r}, E) \) are the macroscopic photon and electron total cross sections, respectively. Equation (1b) is the Boltzmann–Fokker–Planck transport equation, where the third term on the left represents the continuous slowing down (CSD) operator, where \( S_{R}(\vec{r}, E) \) is the restricted collisional plus radiative stopping power. The right-hand side of equations (1) includes the scattering, production and extraneous source terms \( (q^{\gamma} \text{and} q^{e}) \). The scattering and production sources are defined by

\[ q^{\gamma} (\vec{r}, E, \hat{\Omega}) = \int_{0}^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \sigma_{\gamma}^{s} (\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') \Phi^{\gamma} (\vec{r}, E', \hat{\Omega}'), \]  
\[ q^{ee} (\vec{r}, E, \hat{\Omega}) = \int_{0}^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \sigma_{e}^{s} (\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') \Phi^{e} (\vec{r}, E', \hat{\Omega}'), \]  
\[ q^{\gamma e} (\vec{r}, E, \hat{\Omega}) = \int_{0}^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \sigma_{\gamma}^{s} (\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') \Phi^{e} (\vec{r}, E', \hat{\Omega}'), \]  

where \( q^{\gamma} \) is the photon source resulting from photon interactions, \( q^{ee} \) is the electron source resulting from photon interactions and \( q^{\gamma e} \) is the electron source resulting from electron interactions. Here \( \sigma_{\gamma}^{s} \) is the macroscopic photon-to-photon differential scattering cross section, \( \sigma_{e}^{s} \) is the macroscopic photon-to-electron differential production cross section and \( \sigma_{\gamma}^{i} \) is the macroscopic electron-to-electron differential scattering cross section.

The basic assumptions used in equations (1) are briefly summarized as follows. Both charged pair production secondary particles are assumed to be electrons instead of one electron and one positron. Also, the partial coupling technique is assumed, whereby photons produce
electrons, but electrons do not produce photons. The energy from photons produced by the electrons is assumed to be deposited locally. The above assumptions have only a minor effect on the energy deposition field and are similar to those employed in clinical Monte Carlo codes such as VMC++ (Kawrakow 2001). A primary assumption of equation (1b) is that the Fokker–Planck operator (of which the CSD operator is the first-order term) is used for ‘soft’ interactions that result in small-energy losses. Catastrophic interactions that result in large energy losses are represented with the standard Boltzmann scattering.

The macroscopic differential scattering cross section is expanded into Legendre polynomials, \( p_l(\mu_0) \), where \( \mu_0 = \hat{\Omega} \cdot \hat{\Omega}' \). This expansion allows the differential scattering or production cross section(s) to be expressed as

\[
\sigma_{\gamma\gamma/\gamma e/e}^{\gamma\gamma/\gamma e/ee} (\tilde{r}, E', E, \hat{\Omega} \cdot \hat{\Omega}') = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \sigma_{\gamma\gamma/\gamma e/e}^{\gamma\gamma/\gamma e/ee} (\tilde{r}, E') P_l(\mu_0). \tag{4}
\]

Similarly, the angular fluence appearing in the scattering source is expanded into spherical harmonics moments:

\[
\Phi(\tilde{r}, E', \hat{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m}(\tilde{r}, E') Y_{l,m}(\hat{\Omega}), \tag{5}
\]

where \( Y_{l,m}(\hat{\Omega}) \) are the spherical harmonic functions and \( \phi_{l,m}(\tilde{r}, E') \) are the spherical harmonic moments of the angular fluence given by

\[
\phi_{l,m}(\tilde{r}, E) = \int_{4\pi} d\hat{\Omega}' Y_{l,m}^*(\hat{\Omega}') \Phi(\tilde{r}, \hat{\Omega}', E). \tag{6}
\]

where * denotes the complex conjugate. Equations (4) through (6) are exact. Acuros sets a limit on the spherical harmonic order, \( 0 \leq l \leq L \), and hence the number of spherical harmonic moments kept in the scattering/production sources. Using the Legendre addition theorem and the orthonormality of the \( Y_{l,m}(\hat{\Omega}) \), the scattering and production sources become

\[
q_{\gamma\gamma/\gamma e/e}^{\gamma\gamma/\gamma e/ee} (\tilde{r}, E, \hat{\Omega}) = \sum_{l=0}^{L} \sum_{m=-l}^{l} \int_{0}^{\infty} dE' \sigma_{\gamma\gamma/\gamma e/e}^{\gamma\gamma/\gamma e/ee} (\tilde{r}, E') \phi_{l,m}(\tilde{r}, E') Y_{l,m}(\hat{\Omega}). \tag{7}
\]

The upper limit, \( L \), in Acuros is chosen to accurately represent the anisotropy of the scattering source. It was chosen based on previous calculations using a narrow high energy photon beam impinging on a bone-lung slab phantom (Gifford et al 2006). These conditions provided a worst-case scenario, where electron scattering in the bone is highly forward peaked and scattered electrons can travel through a relatively long distance in the downstream lung material. Combined with the small beam size, relatively small differences in the scattering anisotropy can manifest themselves as dose differences in the lung. The results in Gifford et al (2006) showed that \( L = 5 \) was sufficient to provide an accurate solution under these conditions, and this was also used as the maximum value in the current calculations.

Acuros solves equations (1) through discretization in space, angle and energy. In particular, once the electron angular fluence is solved, the dose in any region, \( i \), of the problem may be obtained through the following:

\[
D_i = \int_{0}^{\infty} dE \int_{4\pi} d\hat{\Omega} \frac{\sigma_{eD}(\tilde{r}, E) }{\rho} \Phi(\tilde{r}, E, \hat{\Omega}). \tag{8}
\]

Here, \( \sigma_{eD} \) is the macroscopic energy deposition cross section in units of MeV cm\(^{-1}\) and \( \rho \) is the material density. A benefit of the above approach is that Acuros always calculates the energy-dependent electron fluence everywhere in the computational domain, and thus
dose can be computed as a post-processing quantity. This enables both dose-to-material and dose-to-water to be separately computed from a single transport calculation.

In Acuros, the photon source(s) incident on the patient are represented as point sources, typically located at the treatment head target and possibly at other locations to represent photon scatter, such as below the flattening filter. Each source may have full distributions in both energy and angle, for which source anisotropy may be described by a fluence grid. Such sources allow for the specialized analytic method below to be used to transport the prescribed photon source into the patient anatomy.

For a photon point source, $q_{\gamma}(E, \hat{\Omega})$, located at position $\vec{r}_p$, equations (1) become

\[
\hat{\Omega} \cdot \tilde{\nabla} \Phi^{\gamma} + \sigma_t^{\gamma} \Phi^{\gamma} = q^{\gamma}(E, \hat{\Omega}) \delta(\vec{r} - \vec{r}_p),
\]

\[
\hat{\Omega} \cdot \tilde{\nabla} \Phi^{e} + \sigma_t^{e} \Phi^{e} - \frac{\partial}{\partial E} S_R \Phi^{e} = q^{e} + q^{\gamma e} + q^{e},
\]

where $\delta$ is the Dirac-Delta function. The principle of linear superposition may be used to define the photon angular fluence as the summation of uncollided and collided fluence components,

\[
\Phi^{\gamma} \equiv \Phi^{\gamma}_{\text{unc}} + \Phi^{\gamma}_{\text{coll}},
\]

where $\Phi^{\gamma}_{\text{unc}}$ is the uncollided, or primary, photon angular fluence and $\Phi^{\gamma}_{\text{coll}}$ is the collided, or secondary, photon angular fluence. In this context, primary refers to photons which have not yet interacted with the patient anatomy, and secondary refers to photons which were produced or scattered by a photon interaction in the patient anatomy. Substituting equation (10) into equations (9) and using linear superposition leads to the following system of transport equations:

\[
\hat{\Omega} \cdot \tilde{\nabla} \Phi^{\gamma}_{\text{unc}} + \sigma_t^{\gamma} \Phi^{\gamma}_{\text{unc}} = q^{\gamma}(E, \hat{\Omega}) \delta(\vec{r} - \vec{r}_p),
\]

\[
\hat{\Omega} \cdot \tilde{\nabla} \Phi^{\gamma}_{\text{coll}} + \sigma_t^{\gamma} \Phi^{\gamma}_{\text{coll}} = q^{\gamma}_{\text{coll}} + q^{\gamma}_{\text{unc}},
\]

\[
\hat{\Omega} \cdot \tilde{\nabla} \Phi^{e} + \sigma_t^{e} \Phi^{e} - \frac{\partial}{\partial E} S_R \Phi^{e} = q^{e} + q^{\gamma e} + q^{\gamma e} + q^{e}.
\]

The solution to equations (11) is identical to that of equations (9). However, equation (11a) is decoupled from the other two equations and can be solved independently. Once the solution to equation (11a) is known, $q^{\gamma}_{\text{unc}}$ and $q^{\gamma}_{\text{coll}}$ are formulated and considered fixed sources in equations (11b) and (11c), which then may be solved within the patient anatomy. These sources are generally referred to as the first scattered photon and first scattered electron sources, respectively.

The desired property of equation (11a) is that $\Phi^{\gamma}_{\text{unc}}$ can be solved for analytically. Doing so provides the following expression for the uncollided photon angular fluence from a point source:

\[
\Phi^{\gamma}_{\text{unc}}(\vec{r}, E, \hat{\Omega}) = \delta(\hat{\Omega} - \hat{\Omega}_{\vec{r}, \vec{r}_p}) \frac{q^{\gamma}(E, \hat{\Omega}) e^{-\tau(\vec{r}, \vec{r}_p)}}{4\pi |\vec{r} - \vec{r}_p|^2},
\]

where

\[
\hat{\Omega}_{\vec{r}, \vec{r}_p} = \frac{\vec{r} - \vec{r}_p}{|\vec{r} - \vec{r}_p|},
\]

and $\tau(\vec{r}, \vec{r}_p)$ is the optical distance (measured in mean free paths) between $\vec{r}$ and $\vec{r}_p$, the source and destination points, respectively, of the ray trace.

As previously mentioned, Acuros discretizes in space, angle and energy to solve equations (11a)–(11c). In energy, the energy derivative of the CSD operator in equation (11c)
is discretized using the linear discontinuous finite-element method (Wareing et al. 2001). Energy discretization is performed through the standard multigroup method (Lewis and Miller 1984), used in both the energy dependence of equations (11a) and (11b) and the Boltzmann scattering in equation (11c). In space, Acuros employs a Cartesian mesh using variably sized elements. Commonly referred to as adaptive mesh refinement (AMR), the mesh is limited to refinement in factors of 2 (from one level to the next) in any direction, allowing for localized refinement to resolve areas of sharp gradients. Equations (11b) and (11c), the collision components, are discretized using a linear discontinuous finite-element method, providing a linear solution variation throughout each element, with discontinuities permitted across element faces. The first-scattered-photon and first-produced-electron sources in equation (11a) are also represented as linear varying functions in each element, since these sources are used for the linear discontinuous discretization of equations (11b) and (11c). To obtain the linear variation of these first scattered sources, the analytic solution is computed at spatial quadrature points within each element. The local quadrature order is adapted based on the gradient of the primary photon fluence within the element. Equations (11b) and (11c) are also discretized in angle. The standard discrete-ordinates method is used for both equations, where the angular quadrature order is adaptive by the energy group.

In addition to multiple algorithmic enhancements in Acuros, there are significant differences in how Acuros and Attila discretize the phase-space variables, two of which are discussed here. First, spatial differencing in Attila is performed on a computational mesh consisting of unstructured tetrahedral elements. The mesh is static and is generated prior to the start of the calculation. In Acuros a variably sized Cartesian mesh is employed, with automatic built-in adaptation that increases element refinement near sharp beam gradients and heterogeneities. Secondly, Acuros employs full energy dependence in both the $P_N$ and $S_N$ orders, and allows for variations by particle collision. Both of these features enable a more optimal use of the phase-space variables being solved, providing higher accuracy where it is needed and faster computational times elsewhere.

Acuros problem setup for all the calculations presented below was exactly the same as it was for Monte Carlo simulations. The latter setup is discussed in detail in the next section. Calculated dose matrices were output on the same spatial grid as were Monte Carlo doses. This simplified point-to-point dose comparisons between Acuros and Monte Carlo.

2.1. Monte Carlo simulations

For Monte Carlo calculations we used methods similar to those in our previous study (Vassiliev et al. 2008). Radiation transport and dose tallying were performed with the DOSXYZnrc program (Walters and Rogers 2002). The program is based on the EGSnrc general-purpose Monte Carlo code. It calculates dose distributions in rectilinear geometry for a number of simple sources. We, however, had to write a new source routine that reads a multileaf collimator (MLC) leaf sequence file and samples initial particle direction so that the beam has the shape as is specified in the file. The source routine also takes into account gantry, collimator and couch rotation as well as jaw settings. As in our previous study (Vassiliev et al. 2008), we did not model radiation transport in the accelerator head, including the MLC, because the focus of this study was on radiation transport in the patient. Accordingly, contamination of the beam with electrons produced in the head was not modeled. Additionally, excluding the effects of head scatter, which tend to smooth out incident beam gradients, provides a worst-case scenario for testing the accuracy of in-patient dose-calculation methods. Nevertheless, the beam definitions we applied were realistic enough for the purposes of the study, as comparisons with the Varian standard depth–dose data indicate in figure 1. The agreement is remarkably good, considering
that we did not explicitly model any beamline components such as the flattening filter, or beam contamination with electrons produced in the accelerator head. At 18 MV, however, the model overestimates photon dose in the buildup region. Adding dose from contamination electrons would shift the build-up curve closer to the surface by estimated 2–3 mm. The model is nevertheless acceptable for the purposes of this study, especially considering well-documented difficulties of simulating high energy beams, even with more complex models (e.g. Keall et al (2003)). More specifically, in Monte Carlo simulations the source emitted photons from a point 100 cm from either the phantom surface or a treatment plan isocenter. Initial angular distribution of photons was isotropic. If the initial direction of a particle was such that its projected path entered an area blocked by an MLC or a moveable collimator (jaw), the particle was rejected. Initial photon energy was sampled from a spectrum previously calculated with Monte Carlo using a model of the Varian Clinac 2100 series beamline (Varian Medical Systems, Palo Alto, CA). The model was described and validated in Cho et al (2005) and Vassiliev et al (2006) for 6 and 18 MV beams, respectively. Modeling of a particle history was terminated when its energy fell below 10 keV for both photons and electrons. For the breast treatment plan calculations, a computed tomography (CT) image of an anthropomorphic phantom was converted from a DICOM format to the format of Monte Carlo input files using the CTCREATE program.

The computational domain was voxelized. Absorbed dose was tallied in all voxels. Each voxel contained only one material of a uniform density. For heterogeneous slab phantom calculations most voxels were $2 \times 2 \times 2$ mm$^3$. In the penumbra region the voxel size in the lateral direction was reduced to 1 mm. For the breast treatment plan all voxels were approximately $2.5 \times 2.5 \times 2.5$ mm$^3$. Owing to the simplified beam model we were able to achieve low statistical uncertainties. Since the standard deviation ($\sigma$) varies from voxel to voxel, we report here the median (maximum) standard deviation. This means that in 50% of voxels $\sigma$ was less than the reported median value and nowhere was the reported maximum $\sigma$ exceeded. The standard deviation is given in percent of the local dose. Henceforth in this

![Figure 1](image-url). Depth–dose dependence for 6 and 18 MV 10 × 10 cm$^2$ beams in water. Monte Carlo (solid lines) is compared with the Varian standard data (crosses).
paragraph the word ‘uncertainties’ refers to statistical uncertainties only. For simulations in water phantom (figure 1) the Monte Carlo depth–dose data had uncertainties 0.05% (0.1%) at 6 MV and 0.04% (0.1%) at 18 MV. For the heterogeneous slab geometry depth–dose uncertainties were 0.03% (0.08%) at 6 MV and 0.02% (0.08%) at 18 MV. Uncertainties in profiles at doses greater than 10% of the maximum dose $D_{\max}$ were 0.08% (0.3%) at 6 MV and 0.06% (0.2%) at 18 MV. At doses less than 10% of $D_{\max}$ profile uncertainties were 0.5% (1.4%) at 6 MV and 0.4% (1.4%) at 18 MV. Finally, for simulations of the breast treatment plan in an anthropomorphic phantom the uncertainties in regions where the dose was greater than 5 Gy (10% of prescription dose) were 0.08% (0.3%). For dose regions of less than 5 Gy the uncertainties were 1.1% (8.3%). These latter values are noticeably greater than those we reported for other cases because the treated volume (breast) is a relatively small part of the computational domain covering most of the torso.

### 2.2. Simulated breast treatment

A treatment plan was developed for a custom-designed anthropomorphic phantom (Phantom Laboratory, Inc., Salem, NY) following guidelines and procedures for external beam radiotherapy of breast cancer established at the MD Anderson Cancer Center. A CT image of the phantom was obtained on a GE CT Scanner (GE Medical Systems, Milwaukee, WI) at 2.5 mm slice thickness with the upper body positioned on an incline board. The image was transferred to the Pinnacle3 treatment planning system (v8.0 m, Philips Medical Systems, Andover, MA). A treatment plan was developed using two tangential fields and a field-in-field technique. The prescription was 50 Gy in 25 fractions to the left breast. Both 6 and 18 MV energies were needed to achieve an optimal dose distribution. Most of the dose, 209 out of 238 monitor units, was delivered with 6 MV beams.

Voxel-based material data for both the Acuros and Monte Carlo calculations were derived from the CT image data following exactly the same rules, but different software. The computational domain in the transverse plane covered the entire CT slices. The inferior and superior boundaries were set based on the dose distribution calculated by Pinnacle. The inferior border was 5 cm inferior to the most inferior point of the 10% isodose. Similarly, the superior border was 5 cm superior to the most superior point of the same isodose. This included the entire 1% isodose with a margin. The voxel size was chosen so that the voxel boundaries in the inferior–superior direction coincided with the boundaries of a single CT slice. In the transverse plane each voxel contained $2 \times 2$ CT pixels. For each voxel, the average Hounsfield number of the four pixels was calculated prior to assigning a material to that voxel. Based on this average Hounsfield number, the voxel material was specified to be air, lung, soft tissue or bone, where the Hounsfield number to material conversion was derived based on visual examination of the CT image. The look-up table used for the conversion is given in table 1.

<table>
<thead>
<tr>
<th>Hounsfield units range</th>
<th>Material</th>
<th>Density (g cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Less than −853</td>
<td>Air</td>
<td>$1.2048 \times 10^{-3}$</td>
</tr>
<tr>
<td>From −853 to −154</td>
<td>Lung</td>
<td>0.26</td>
</tr>
<tr>
<td>From −153 to 101</td>
<td>Soft tissue</td>
<td>1</td>
</tr>
<tr>
<td>Greater than 101</td>
<td>Bone</td>
<td>1.85</td>
</tr>
</tbody>
</table>
3. Results and discussion

3.1. Slab phantom

Depth–dose curves along the central axis of the heterogeneous phantom were calculated for 6 and 18 MV photon beams, and field sizes 2.5 × 2.5, 5 × 5 and 10 × 10 cm² (figures 2 and 3). For better clarity in these and in other figures of this type we omitted some Acuros data points where they were too dense. For 6 MV fields at depths of 1–30 cm, maximum relative differences between Acuros and Monte Carlo were less than 1.5% (local dose difference) for all voxels. If differences are based on a percentage of the maximum dose ($D_{\text{max}}$) as is commonly done, the maximum voxel differences were less than 1.2%. In the build-up region of the 6 MV field (beam depths of 0–1 cm), the distance to agreement (DTA) was calculated and did not exceed 0.7 mm for any tested voxels. For 18 MV fields at depths of 2–30 cm, the maximum relative difference between Acuros and Monte Carlo voxels was 2.3%, which was located in the lung region of the 2.5 × 2.5 cm² field. If results were compared as a percentage of $D_{\text{max}}$, the maximum difference would be 1.5%. For all other fields, the maximum relative differences were less than 1.7%, or 1.1% of $D_{\text{max}}$. In the build-up region of the 18 MV field (beam depths of 0–2 cm), the DTA was less than 0.3 mm for all tested voxels.
Figure 3. The same as in figure 2 for 18 MV beams. Two curves are shifted by $\pm 0.3 \times 10^{-12}$ Gy · cm$^2$ MeV$^{-1}$ as indicated by the arrows.

Figure 4. Lateral dose profiles for a 6 MV beam in a heterogeneous slab phantom. Phantom size is $30 \times 30 \times 30$ cm$^3$, distance from the source to the phantom surface is 100 cm, field sizes are $2.5 \times 2.5$ cm$^2$ and $10 \times 10$ cm$^2$ at the phantom surface, depths are 1.5, 10 and 20 cm.

Lateral dose profiles were compared for all three field sizes: $2.5 \times 2.5$, $5 \times 5$ and $10 \times 10$ cm$^2$. Depths of 1.5, 10, 20 cm were compared for the 6 MV fields, and depths of 3.5, 10, 20 cm for the 18 MV fields. The $2.5 \times 2.5$ and $10 \times 10$ cm$^2$ profiles are shown in figures 4 and 5. For all voxels where the dose was greater than 10% of $D_{\text{max}}$, the local relative dose differences between Acuros and Monte Carlo was evaluated. For low dose regions where the
dose in voxels was less than 10% of $D_{\text{max}}$, differences were evaluated based on the percentage of $D_{\text{max}}$.

For all voxels in all profiles of the 6 MV fields where the dose was greater than 10% of $D_{\text{max}}$, maximum differences between Monte Carlo and Acuros were within 1% or 1 mm DTA, except in the $5 \times 5$ cm$^2$ field, where maximum differences were within 2% or 0.3 mm DTA. For all voxels in all profiles of the 6 MV fields where the dose was less than 10% of $D_{\text{max}}$, maximum differences between Monte Carlo and Acuros were within 1.0% of the maximum dose, $D_{\text{max}}$.

For all voxels in all profiles of the 18 MV fields where the dose was greater than 10% of $D_{\text{max}}$, maximum differences between Monte Carlo and Acuros were within 1% or 1 mm DTA. For all voxels in all profiles of the 18 MV fields where the dose was less than 10% of $D_{\text{max}}$, maximum differences between Monte Carlo and Acuros were within 0.4% of $D_{\text{max}}$.

3.2. Anthropomorphic phantom

Figure 6 shows isodoses for the breast treatment plan in an axial plane through the isocenter. The Acuros and Monte Carlo results are compared at isodose levels of 5, 25, 50 and 52 Gy. The maximum dose in this plane was 53 Gy. As shown, results from both codes are in close agreement. A more quantitative comparison is provided in figure 7, where isodose contours are shown for local dose differences between Acuros and Monte Carlo, at 2, 5 and 10%. As indicated, differences are predominantly in the air external to the patient and in the lateral penumbra on the inside edge of the fields. The differences in the penumbra are in a high gradient region and have a small DTA. This is illustrated in figure 8, where only eight voxels failed the 2%/1 mm DTA criteria in the axial plane through isocenter. In this plane, 0 voxels failed the 2%/2 mm DTA criteria. Figures 9 through 11 present line plot comparisons between Monte Carlo and Acuros along three different directions.

In the 3D volume, 77 576 voxels were evaluated for agreement, which consisted of those voxels within the patient and where the dose was greater than 5 Gy ($\sim$10% of $D_{\text{max}}$). Out of these voxels, 1047 voxels failed the 2%/1 mm DTA criteria and 98 failed the 2%/2 mm DTA criteria.
Figure 6. Isodoses for the breast treatment plan in an axial slice through the isocenter. Acuros isodose curves are shown in different colors as indicated in the graph, with Monte Carlo isodose curves shown in white. The latter are almost entirely covered by their respective Acuros isodoses, especially at 25 Gy.

Figure 7. Contour plot of dose differences between Acuros and Monte Carlo in an axial slice through the isocenter. The dose difference for each voxel is scaled by the local dose (i.e. dose in the same voxel), instead of $D_{\text{max}}$. Data only for voxels in which the dose is greater than 5 Gy are shown.

criteria. This corresponds to 98.7% voxels passing the $2\%/1\,\text{mm}$ DTA criteria and 99.9% passing the $2\%/2\,\text{mm}$ DTA criteria.

For all cases, Acuros calculation times were less than 5 min on a workstation with two dual-core AMD Opteron processors. Although a direct comparison between Attila and Acuros
Figure 8. Plot showing voxels (red) in an axial slice through the isocenter where differences between Acuros and Monte Carlo are greater than 2% or 1 mm DTA. The dose difference for each voxel is based on the local dose (i.e. dose in the same voxel), instead of $D_{\text{max}}$. Data are shown only for voxels in which the dose is greater than 5 Gy. The isocenter is at the intersection of the two green lines.

Figure 9. Dose profile in the left–right direction along a line through the isocenter. The line is shown in green in figure 8. The profile ends where the line enters a low dose region or air outside the phantom.

was not performed in this study, for a prescribed level of accuracy, the version of Acuros in the present study is roughly an order of magnitude faster than Attila. A previous study was performed using Attila for both head-and-neck and prostate case, where calculation times of
19.6 and 16.1 min, respectively, were reported on a single 2.2 GHz AMD processor (Vassiliev et al 2008). For these cases, accuracy was evaluated based on the 3%/3 mm DTA criteria. This is much less stringent than the present study, where Acuros agreed with Monte Carlo to within 2%/1 mm DTA. As these studies indicate, a high sensitivity exists between the calculation speed and accuracy. In Monte Carlo this trade-off also exists; when fewer particles are tracked, statistical noise increases. In GBBS methods such as Acuros and Attila, errors are systematic and increase with faster calculation times. However, in the Attila study, the
3%/3 mm criteria is still clinically relevant. This indicates that Acuros may be well suited for optimization, where rapid calculation times are desired with clinically relevant accuracy.

4. Conclusions

In this study, detailed comparisons were made between Acuros, a GBBS and Monte Carlo in the presence of significant heterogeneities. GBBS and Monte Carlo methods both solve the Boltzmann transport equation through different approaches. Although different methods may be employed for resolving the soft collisions of electrons, the achievable accuracy of both methods is otherwise equivalent. The results of this study support this conclusion, as an excellent agreement between both Acuros and Monte Carlo was obtained. Nevertheless, it is important to cover in future studies a broader range of clinically relevant cases, perhaps focusing on those that may present computational challenges such as localized heterogeneities in the field, small fields, sharp edges and high density gradients.

The clinical viability of a dose-calculation method is based on its combination of speed and accuracy. All existing clinical methods have their limitations, and significant room for improvement exists. Although pencil-beam convolution methods are generally fast, accuracy is known to be compromised especially in the presence of heterogeneities. More sophisticated model-based algorithms, such as collapsed-cone convolution, can provide improved accuracy but at the expense of longer calculation times. Although Monte Carlo methods are widely recognized as providing superior accuracy, long calculation times and statistical noise limit their clinical usefulness.

The recent growth in arc therapy treatments, which use a large number of beams, has provided a computational challenge to historically fast algorithms, such as pencil-beam and convolution superposition. Since calculation times for these algorithms generally scale linearly with the number of beams, lengthy calculation times can result for arc therapies. Since calculation times for Acuros are only weakly dependent on the number of beams, Acuros has the potential to provide both high accuracy and fast calculation times in a single dose-calculation engine.

Acknowledgment

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