



# A time-dependent neutron transport method of characteristics formulation with time derivative propagation



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## ABSTRACT

A new time-dependent Method of Characteristics (MOC) formulation for nuclear reactor kinetics was developed utilizing angular flux time-derivative propagation. This method avoids the requirement of storing the angular flux at previous points in time to represent a discretized time derivative; instead, an equation for the angular flux time derivative along 1D spatial characteristics is derived and solved concurrently with the 1D transport characteristic equation. This approach allows the angular flux time derivative to be recast principally in terms of the neutron source time derivatives, which are approximated to high-order accuracy using the backward differentiation formula (BDF). This approach, called Source Derivative Propagation (SDP), drastically reduces the memory requirements of time-dependent MOC relative to methods that require storing the angular flux. An SDP method was developed for 2D and 3D applications and implemented in the computer code DeCART in 2D. DeCART was used to model two reactor transient benchmarks: a modified TWIGL problem and a C5G7 transient. The SDP method accurately and efficiently replicated the solution of the conventional time-dependent MOC method using two orders of magnitude less memory.

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## 1. Introduction

We are in the midst of a transition in the state-of-the-art for reactor kinetics. Until recently, reactor transients have been principally modeled using the diffusion approximation to the transport equation [1]. While diffusion methods are computationally efficient, there is growing interest in reactor designs and fuels for which diffusion may not be sufficiently accurate. Consequently, there is interest in the direct use of neutron transport methods for nuclear reactor kinetics [2–8], and this is increasingly practical due to the steady advances in computational power.

Method of Characteristics (MOC) [9,10] is a popular method for solving the steady-state neutron transport equation, especially for small, assembly-level models. Its popularity stems from its ability to resolve complex geometry without spatial homogenization. As with other transport methods, it has been extended to solve the time-dependent transport equation as well.

Most reactor kinetics methods in neutron transport and diffusion treat time dependence by discretizing the equations in time and applying a conventional time integration method to approximate the time derivative (e.g. Backward Euler, Theta Method, Runge–Kutta, etc.). In this case, the spatial and angular dependence are treated using the same approach that would

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be employed to solve the steady-state transport equation (e.g. PN, SN, MOC, etc.). The result is that the time-dependent transport problem is reduced to a series of pseudo-steady-state problems at discrete points in time coupled to previous time points through the update of state variables and the treatment of the time derivatives. This approach is used in many time-dependent neutron transport codes, including the three-dimensional whole core neutron transport code DeCART [4,11,12] which was used in this work.

One obstacle with this approach is that it implies that the neutron angular flux<sup>1</sup> should be stored from one or more previous time steps in order to represent the angular flux time derivative. Although the angular flux is the fundamental solution of the transport equation, the neutron scalar flux<sup>2</sup> is often the desired solution in practice. The scalar flux is the integral of the angular flux over all angles in space, and it is generally used to calculate reaction rates. Thus in steady-state transport the angular flux is not generally stored; it is instead numerically integrated as it is generated to calculate the scalar flux. Storing the angular flux for large reactor models requires staggering amounts of memory that can exceed the capabilities of even leading-class supercomputers. As a result, time-dependent neutron transport codes are either very limited in the size or resolution of the reactor transients they can model, or they employ low-order angular or spatial approximations to treat the angular flux time derivative.

To circumvent the angular flux storage issue, we investigated an alternative class of time-dependent transport methods called time-derivative transport, whereby a transport equation is derived for the angular flux time derivative and simultaneously solved with the transport equation for the angular flux. When this concept is applied to MOC, the angular flux time derivative is solved by propagation in terms of the neutron source<sup>3</sup> time derivatives. As a result, we call this method Source Derivative Propagation (SDP).

One significant advantage of SDP is that it can be inexpensively extended to high-order accuracy by approximating the source time derivatives using the Backward Differentiation Formula (BDF). By contrast, if BDF is applied directly to the angular flux time derivative for time-dependent MOC, the memory problem is significantly exacerbated. For the problems examined in this work, SDP method with high-order BDF approximations to the source derivatives accurately replicated the conventional, high-order time-dependent MOC solution when the same BDF order and time steps were used.

Other researchers have also recently investigated angular flux time derivative approximations for time-dependent MOC. Talamo developed three conventional time-dependent MOC formulations which represent the current practice for time-dependent MOC [7]. Talamo's Method II stored the angular flux to represent the time derivative while Methods I & III approximated the time derivative using the scalar flux. Method II is equivalent to our reference method for assessing the accuracy of SDP while Method I is equivalent to our reference method for assessing computational efficiency. While Talamo observed that the methods that approximated the time derivative as isotropic were generally accurate, Method I was unstable with very short time steps. This instability was not observed in this work because we did not require such small time steps.

In contrast to Talamo, Tsujita addressed the angular flux memory issue by developing a time-dependent MOC formulation that recalculated the previous angular fluxes on the fly [8]. While in principle this could be done for an arbitrary number of time steps, with each successive time step the method becomes linearly more computationally expensive. To limit this expense, Tsujita only recalculated the angular fluxes for a few previous time steps and used an isotropic approximation for the earliest recalculated time step. While the isotropic approximation introduces some error, the error is mitigated because with each earlier time step recalculated on the fly, the error term is multiplied by an additional inverse-velocity term, which is very small. While the derivation of Tsujita's on-the-fly (OTF) method is very different from the SDP method explored in this work, it has similar computational and memory requirements. The primary advantage of SDP over OTF is that SDP is more inexpensively extended to high-order accuracy in time using BDF.

A high fidelity alternative to applying a finite differencing technique to treat the angular flux time derivative for time-dependent MOC is to map the characteristics to the time domain as well as the spatial domain. This space-time transport is in principle very accurate because it explicitly accounts for neutron time of flight, but it is substantially more computationally expensive and memory intensive than methods like SDP and OTF. Pandya and Adams developed a 3D space-time MOC method for radiative transfer using this approach [13], while Tsujita et al. implemented a 1D space-time MOC method for reactor kinetics [14]. We originally developed the early SDP methods using a space-time characteristic formulation with coarse approximations in the time domain [15]; the derivation presented in this work is equivalent but more succinct.

In Section 2 we will provide the time-dependent MOC formulations used in this work, including SDP. Section 2.1 will briefly present two conventional time-dependent MOC methods which are representative of the state of the art. In Section 2.2 we will derive the primary SDP method used in this work. Other SDP methods were evaluated in [16]. In Section 3 we will present two reactor transient benchmark problems: a comparatively simple TWIGL problem [17] and a more challenging C5G7 transient [18]. After presenting each benchmark problem we will assess the accuracy and efficiency of the SDP method by comparison to the reference methods. A summary and conclusions are presented in Section 4.

<sup>1</sup> The neutron angular flux is the solution of the neutron transport equation and is defined as the instantaneous neutron path rate density in space, angle, and energy.

<sup>2</sup> The neutron scalar flux is the neutron angular flux integrated over all directions. The scalar flux is of interest to nuclear reactor engineers because it is used to calculate nuclear reaction rates.

<sup>3</sup> In many neutron transport methods, the neutron source terms (e.g. fission, decay, etc.) are combined into a single term which is updated iteratively.

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