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14. ABSTRACT

Nonequilibrium radiative heat transfer becomes a technical limiter to thermal protection for high-performance aerospace vehicles due to the deficient modeling and simulation capability. The complex radiative simulation must be built on the interaction of quantum physics, chemical kinetics, aerodynamics, and radiation transfer. The most efficient and accurate approach in solving the nonequilibrium radiative energy transfer equation is based on statistical mechanics by ray tracing (Monte Carlo) method. In this approach, the required spectral properties of a chemically reacting gas for radiative evaluation are interpolated from the computational results from the nonequilibrium flowfield and mapped onto the emitting/absorbing electromagnetic wave paths. The present research effort has created a space partition algorithm for the nearest neighbor search optimization on both structured/unstructured grids and integrated with the high-resolution orthogonal polynomial refinement technique for this multi-disciplinary science. Through the computational mathematics basic research, a systematic ray-tracing method jointly applied with the line-by-line spectral computations is now practical. Meanwhile, an even more efficient computational algorithm adopting the view-factor approach for radiative energy transfer in axisymmetric hypersonic flows has also been successfully accomplished. The resultant research efforts open a new research avenue for others to follow and to bring a new level of performance to the multi-disciplinary modeling and simulation capability for nonequlibrium radiation.

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Simulating Nonequilibrium Radiation via Orthogonal Polynomial Refinement
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Analysis

The complex nonequilibrium radiative simulation for high-speed flow is built on the interlocking phenomena between quantum physics, aerodynamics with nonequilibrium chemical reaction, and radiation transfer. All dominant chemical-physical phenomena are occurred at the molecular/atomic scales and all radiative energy transfers are also taken place at the quantum transitions of internal degrees of freedom by molecules or atoms, thus the phenomenon must be modeled [1-4]. In addition, the chemical species concentrations and its associated thermodynamic states of an inhomogeneous flowing medium are solved on a coordinate system according to the flowfield structure. On the other hand, the radiation energy transmission follows the line-of-the-sight path of electromagnetic waves [5,6]. Therefore, two intrinsically different coordinates are required to simulate simultaneously the multi-disciplinary phenomenon. Meanwhile the spectral properties such as the emission and absorption are exclusively tied to the local thermodynamic state and compositions of the flow medium. The required optical parameters for the nonequilibrium phenomena simulation need to be determined from data bases which are derived from quantum physics and transmit across the two different coordinates by a nearest neighbor search algorithm [7,8].

An accurate and efficient computational capability for nonequilibrium radiation simulation via the ray tracing technique has been accomplished [9,10]. The radiative rate equation is fully coupled with the aerodynamic conservation laws including the finite-rate chemical and chemical-physical kinetic models [3,4]. The interdisciplinary governing equations are solved by an implicit delta formulation via the diminishing residual numerical scheme. For physical validation, the axisymmetric radiating flowfield over the reentry RAM-CII probe is first simulated and verified with flight data and previous solutions by traditional CFD methodology for nonequilibrium reacting flows [11]. The transport properties are determined by kinetic theory of diluted gas, and the radiative emission and absorption coefficients are then obtained by electronic databases as well as approximate quantum chemical-physics *ab-initio* computations. These data are then mapped onto the radiating wave path for radiative energy transfer.

In order to achieve a spectral-like numerical accuracy, the high-gradient domain within the shock layer is resolved by applying the local high-resolution orthogonal polynomial refinement technique [12]. Through which the rapid rates of changes by dependent variables are generated by the Gauss-Lobatto quadrature formulation with grid density clustering on the roots of the Legendre polynomial. Two special properties of the Gauss-Lobatto quadrature for high resolution are that the solution is exact on these root points by the divided difference interpolation formula or the Cardinal function, and the first derivative has the accuracy of the n^{th} order polynomial. The numerical solutions are attained an unprecedented physical fidelity in comparing with all previous computational simulations.

Another innovation is the space partition algorithm (SPA) created by the research effort for the interpreting process between the different frames of references through the nearest neighbor search or the commonly referred to as the proximity search. It is an optimization problem for locating the closest discretized grid points among the two coordinates in metric space. The performance of nearest neighbor algorithms is usually measured by the preprocessing time, computer memory space, and average query time. In many search procedures for the number of points n_p of a data set, a fast algorithms require preprocessing time to be scaled by $O(n_p log n_p)$, with a n_p storage space and to achieve $O(log n_p)$ mean query time. However, a common conclusion from nearly all NNS research shows the performance of NNS algorithm varies greatly with the properties of the data set. Therefore, the improved efficiency by the present study is limited to the one-on-one comparison of the traditional approach and the space partition algorithm on an identical data set [7,8]. The interrogating process for the query points by space partition algorithm becomes unnecessary and the search space is completely defined by the vector projection of the surface outward normal.

The structured grid topology permits a vastly reduced searching space for the NNS along all radiating rays. On a structured grid, the search domain in the meridian plane is bounded by the surface point $\vec{r}_b(x_b, y_b, z_b)$ from which a radiating ray originated and the interception of this ray at the outer boundary $\vec{r}_o(x_o, y_o, z_o)$. In Figure 1, the reduced NNS searching space by the process of elimination is illustrated: The searching domain is drastically reduced and limited to the bounded space between the body surface and the enveloping shock wave. The search process of SPA excludes a huge data domain above and below the tracing ray. Equally important, this algorithm for the search space is also automatically bypassing the data interrogating preprocess for NNS. The algorithm for defining the reduced search domain in three-dimensional space of the SPA is simply defined by the coordinate indices;

$$1 < i < i_o$$

$$j_b - 1 < j < j_o + 1$$

$$k_b - 1 < k < k_o + 1$$

On a structured grid, the required data interrogating preprocess by NNS is completely eliminated by the SPA, and the search is conducting in a vastly reduced data space defined by these indexes. On an unstructured grid, this process can be further facilitated by the intrinsic next-neighbor-connectivity construction as depicted in Figure (2). Once a query point is determined, the search along a tracing ray will proceed to the next neighbor cell in the search space.

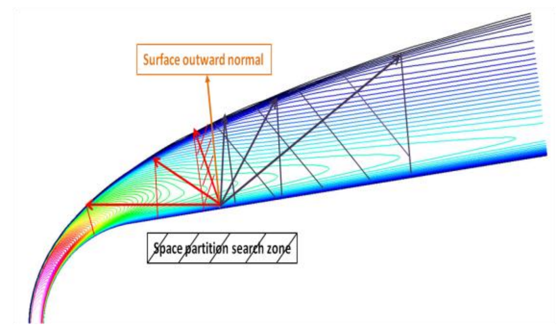

Figure 1. Reduced Nearest Neighbor Search space by the surface outernormal vector, (red hatched domain along tracing ray)

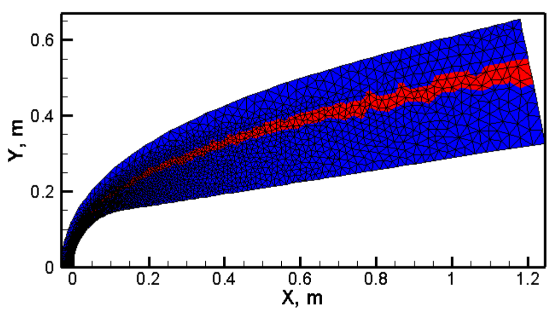

Figure 2. Search domain by the next-neighbor-Connectivity for unstructured

Two unique features of the present approach have been successfully implemented to achieve a new capability for the interdisciplinary computational simulation. The space partition algorithm for the nearest neighbor search process combining with the better placement of the query points along the tracing rays by the Gauss-Lobatto polynomial has demonstrated more than one-order-of-the-magnitude improvement to the computational efficiency for the nonequilibrium radiating hypersonic flow by the conventional methodologies. On the relatively small data bases of 15,416 and 60,636 discrete points, the factors of 20.82 and 44.38 times in computational efficiency gain are realized over the existed procedure.

Grid distribution/Algorithm	Equal space/ Brute search	Gauss-Lobatto/Space Partition
CPU Time , s	1321.14	29.77
Radiation Flux, W/cm^2	7.6095×10^{-2}	7.6070×10^{-2}
Query points along each ray	800	150
Number of data base	60,636 (326x186)	60,636 (326x186)
Number of tracing rays	3721 (61x61)	3721 (61x61)

A more than forty times computational efficiency gain is achieved from the integrated space partition algorithm for the nearest neighbor search optimization and optical data interpolation from the nonequilibrium flowfield, as well as, the local resolution refinement through the Gauss-Lobatto polynomial.

In the final phase of the basic research project is focused on the development of the view-factor approach to the nonequilibrium radiation simulation. The key idea of this approach is to establish a visible factor between the elements participating in the radiative energy exchange while the non-participating elements is defined by an solid angle in which the emitting element is observed by the receiving elements. When the gas medium between exchanging elements have their own radiative properties, the radiative attenuation is included in the definition of the view factor [13]. The geometry of the participating elements can take very general appearance and establishes for the volume-to-volume type of energy exchange. According to the concept of photon propagation along the line of sight between emitting and receiving elements, this approach is overlapping to the ray-tracing method [2,3,9].

In general, it is not possible to achieve a three-dimensional analytic form for the view factor because the temperature and optical path is varying with the azimuthal angle. Thus the radiation flux density must be calculated by direct numerical integration. However when the flowfield is axisymmetric and the propagation of electromagnetic wave in a non-scattering but emitting and absorbing medium, a semi-analytic expression for the radiative flux density is possible by the commonly accepted local thermal equilibrium (LTE) approximation. A semi-analytic expression for the radiative flux density has been derived and verified by a direct comparison of computational results. The computational efficient view-factor approach in an optically thin medium describing by the realistic multi-group optical model is demonstrated in Figure 3 by comparing with the previous results from the ray-tracing method. It is observed that the view-factor approach can attain comparable computational accuracy to that by the more rigorous ray-tracing method and yields superior results than the widely adopted tangent slab approximation.

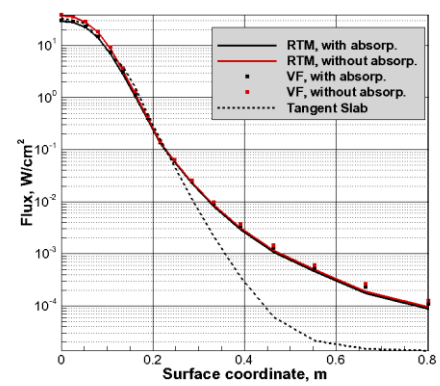

Figure 3. comparison of ray-tracing , view-factor, and tangent slab methods for RAMC-II reentry probe at altiude of 61 km

The research results have developed a tier-structure computational modeling and simulation procedure for analyzing nonequilibrium radiation phenomena in hypersonic flight environment. The research accomplishments are published in eight (8) articles in international/national journals and disseminated to sixteen (16) national conferences. A direct technologic transfer has also taken place in supporting AFRL/RQ mission for high-performance combustion chamber evaluation by a Task Order 0004, FA8650-08-D-2806.

Acknowledgment/Disclaimer

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Publications

Journal articles

1. Shang, J.S. and Surzhikov, S.T., Simulating Stardust Earth Reentry with Radiation Heat Transfer, J. of Space craft and Rockets, Vol. 48, No. 3, 2011, pp.385-396.
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Honors & Awards Received

USAF Basic Research Award, 1986
Fellow of AIAA, 1993
AIAA Plasmadynamics and Laser Award, 2004
Keynote Speaker, 4^{th} International Symposium on Jet Propulsion and Power Engineering. 2012

AFRL Point of Contact

Dr. Richard Rivir, AFRL/RQ WPAFB, OH 937-656-2810, actively interacted on FA8650-08-D-2806 Task Order 0004; Path-finding study for radiative exchange in combustion chamber.
Mr. Frank Witzeman, AFRL/RQV WPAFB, OH 937-255-6156, interacted and met weekly.

Dr. Melvyn Roquemore, AFRL/RQT WPAFB, OH 937-255-6813
Dr. Roger Kimmel, AFRL/RQH WPAFB, OH 937-255-8295, interacted weekly.

Transitions

The present research was initiated to introduce innovative numerical algorithms and to develop high-resolution simulation capability for basic research on the nonequilibrium radiative heat transfer. Based on this long-term objective, the technical transitions are focused on the disseminated of research results first to the research scientists of AFRL and then to national/international conferences of professional societies. The technical transition processes are consistently followed up through personal interactions.

A path-finding study for radiative energy exchange in combustor chamber was established on October 2012 by the AFRL/RQ of the Task Order 0004, FA8650-08-D-2806 through United Technology Incorporated of Dayton with the principal investigator, Prof. J. Shang of Wright State University. This task is planned to address the increasingly challenging thermal protection requirement for high stagnation pressure condition within the combustion chamber. This technical requirement represents the most effective technical transition between the AFOSR funded university research in direct support to AFRL technical Directorate.

The concept and potential practical applications of the Gaussian quadrature to premixed- and non-premixed turbulent hydrogen combustion has exchanged with Dr. W. Melvyn Roquemore of the Aerospace System Directorate of Air Force Research Laboratory (AFRL/RQT 937-255-6813). A continuous exchange and collaboration has been maintained with the combustion research group AFRL/RQT. This activity has proved to be extremely mutual benefit in advancing basic understanding of extremely complex combustion phenomena for USAF's interest.

New Discoveries

None.