Reduced-order Non-equilibrium Radiative Transfer for 3D Problems

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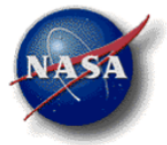
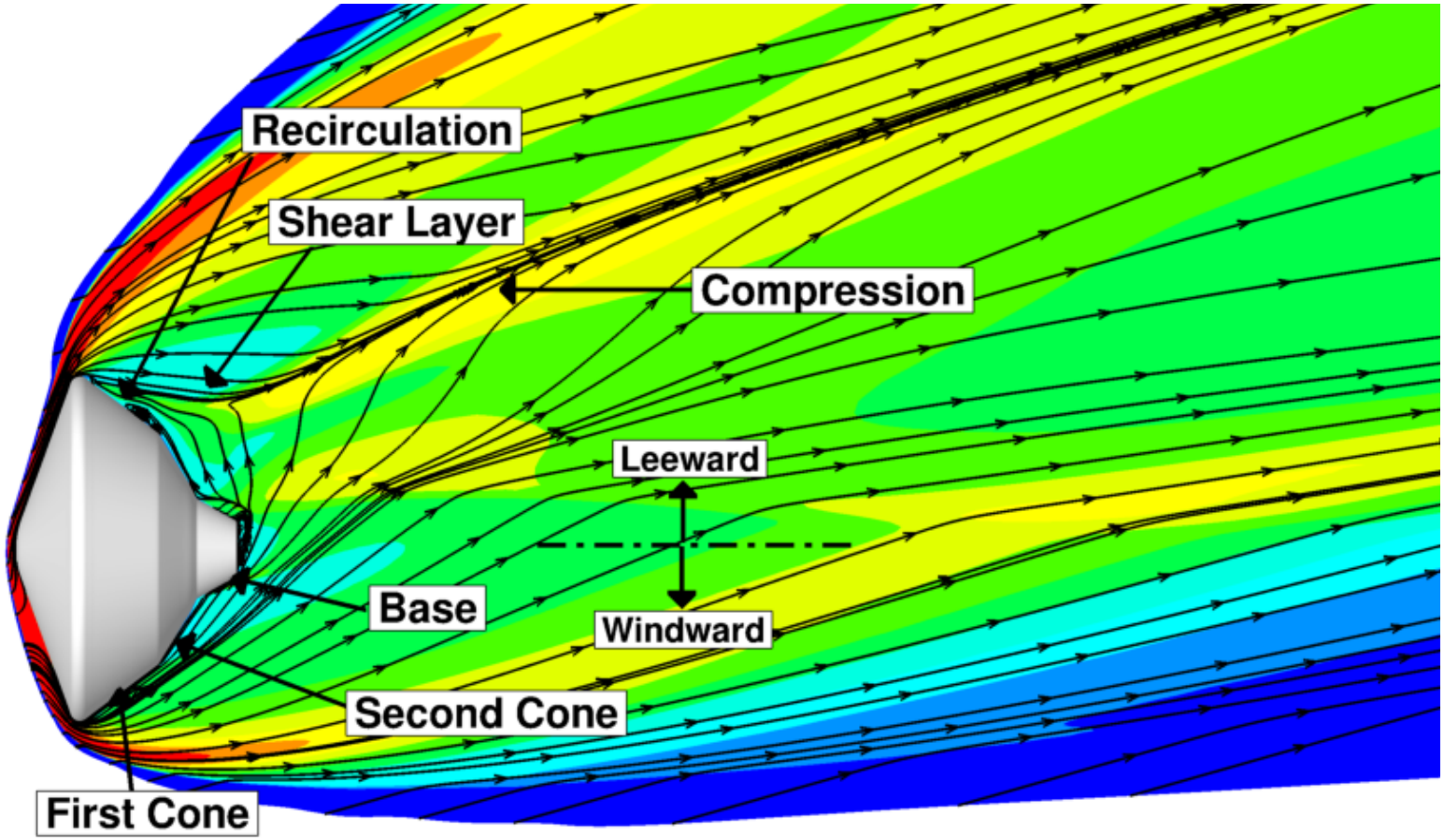


Outline

1. Introduction
2. Spectral Reduced-order Models
3. Radiation Binning Strategy
4. 3D RTE
5. Mars Entry Wake Flows
6. Summary and Future Work

Introduction

- Coupled flow-radiation calculations crucial for accurately characterizing properties for different applications:



Hypersonic Planetary Entry

Sahai *et al.*, AIAA Scitech 2019.

Introduction

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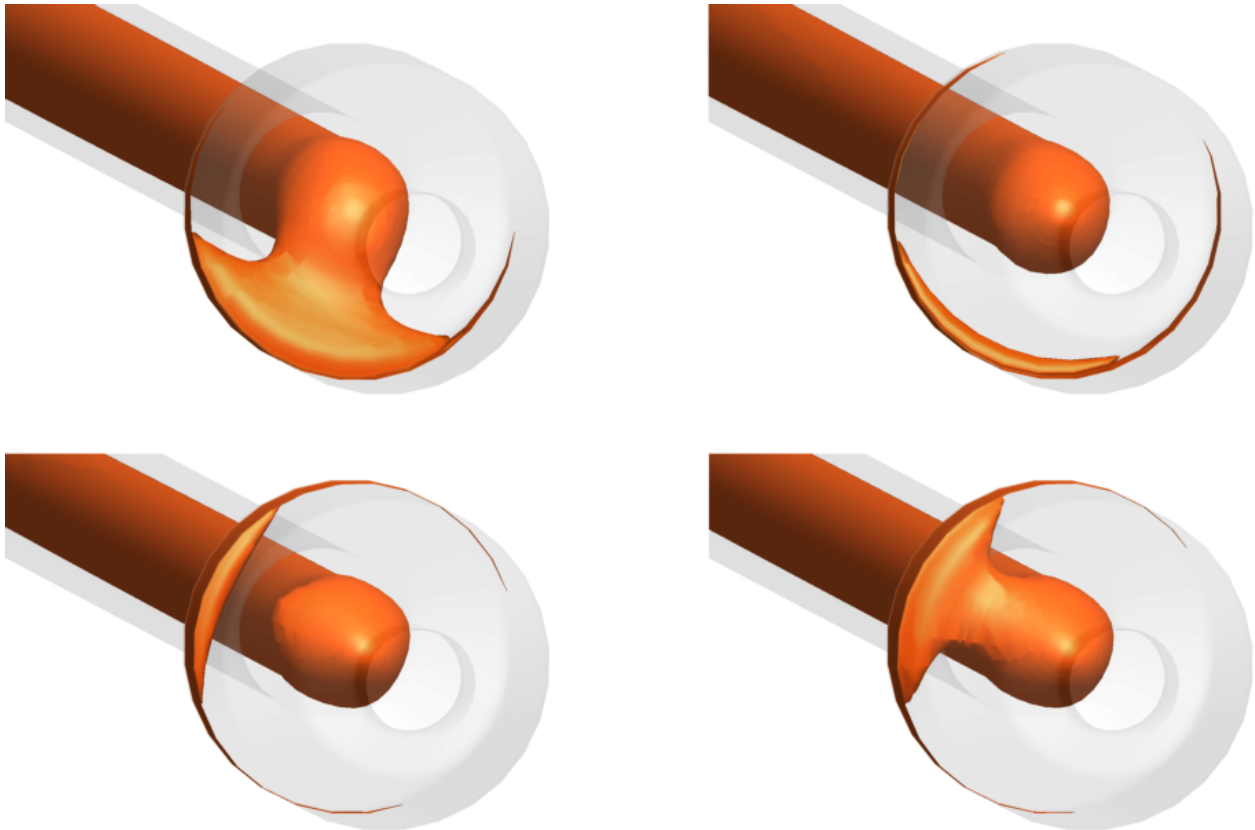

Arc-heated Flows

Sahai *et al.*, Plasma Sources Science and Technology 2017.

Introduction

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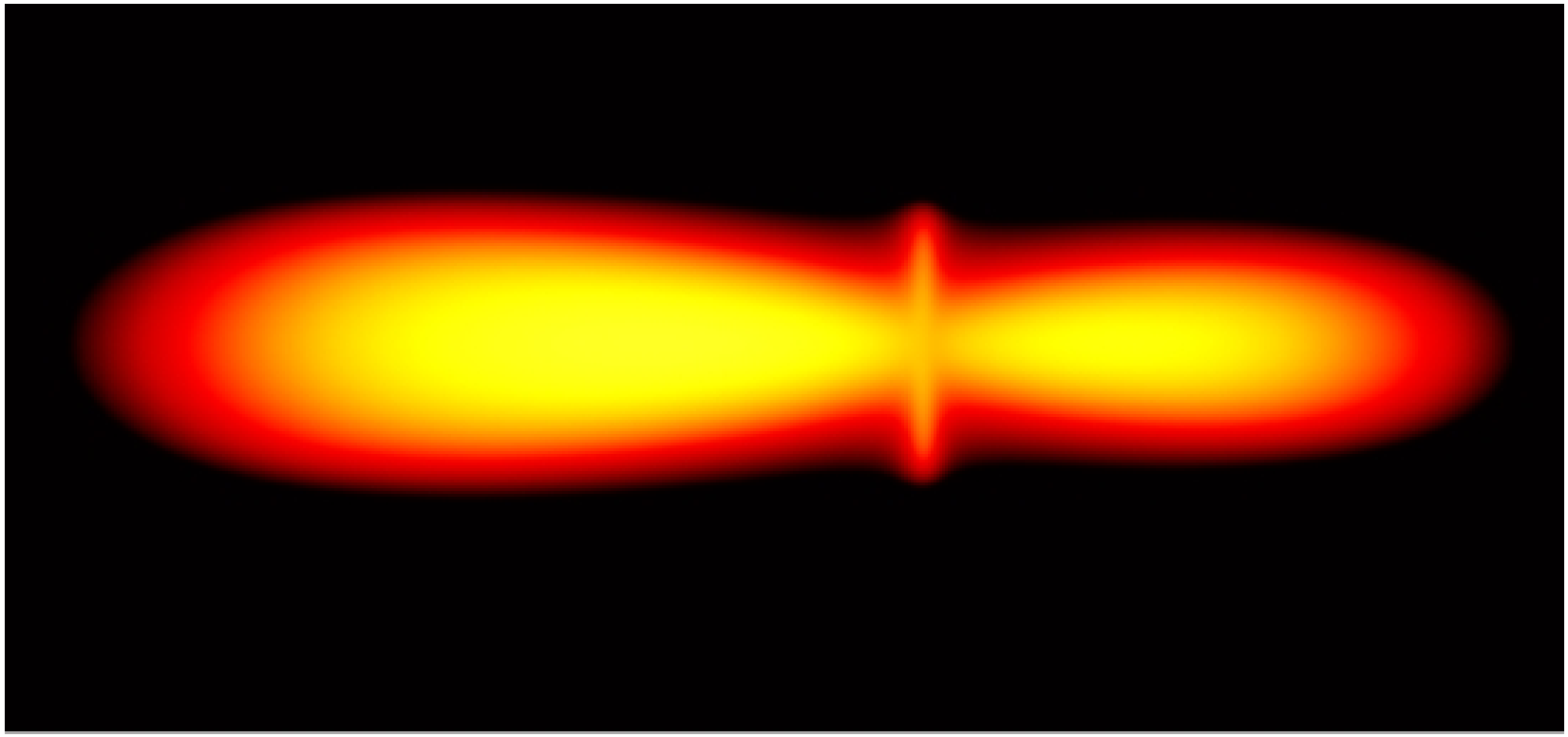
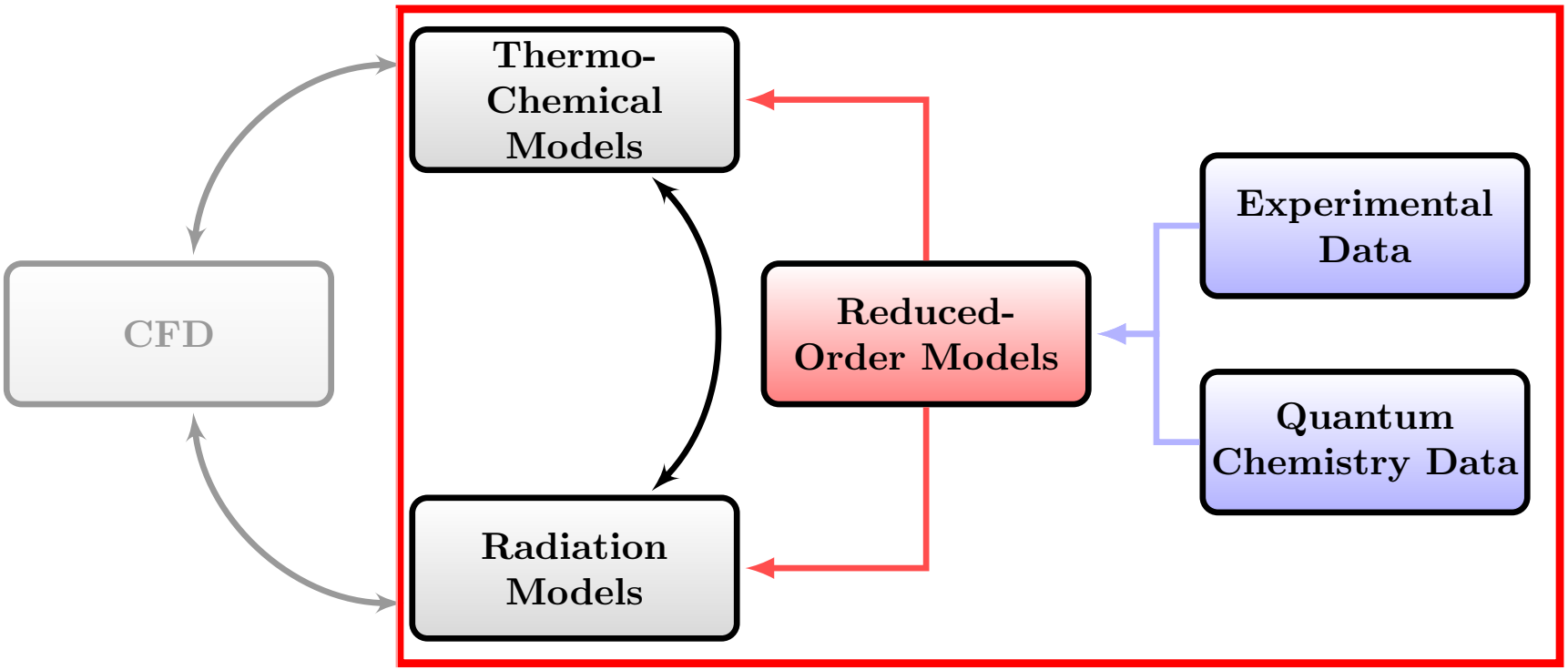


Laser-plasma Interaction

Alberti *et al.*, AIAA Scitech 2019.

Objective

"Development of a physics-based reduced-order framework for solving non-equilibrium chemical kinetics and radiation for complex flow problems."



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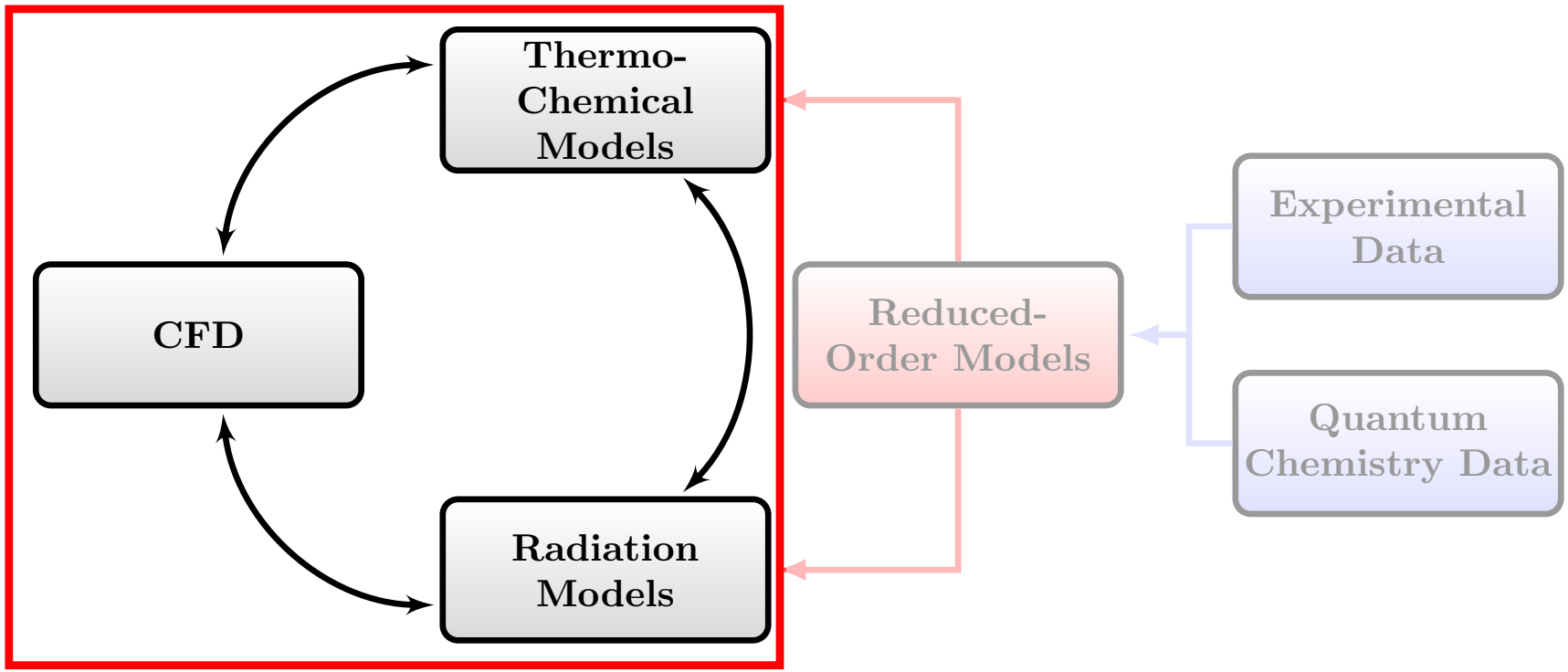
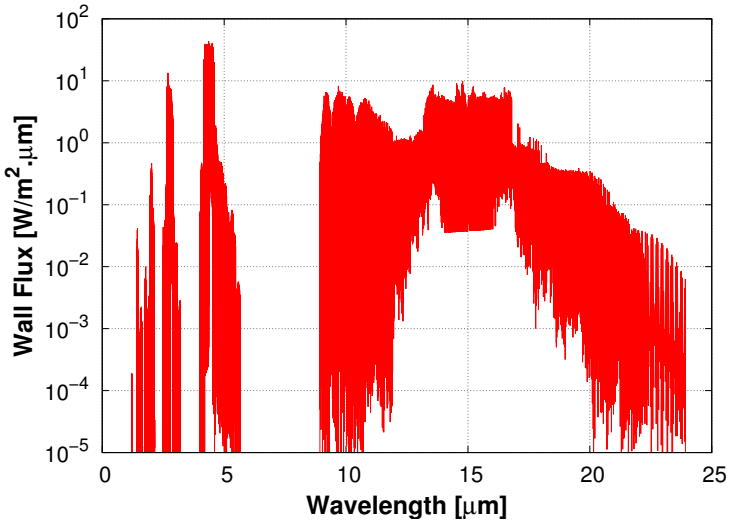


"Model-reduction imperative for resolving two-way coupling between thermochemical and radiation models."

Objective

- **Three key challenges** for performing radiation calculations in conjunction with CFD:
  - Evolve efficient / accurate reduced-order models to capture spectral variance in properties.



Spectrally varying radiative wall heat flux from CO_2 for a 1-D problem

  - Solve radiative transfer equations (RTEs) for 3D unstructured meshes.
  - Self-consistent radiation-flow coupling to account for non-local absorption.

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Reduced-order Models for Spectral Properties

- Monochromatic steady-state RTE describing the spectral intensity I_ν corresponding to frequency ν in the $\mathbf{\Omega}$ direction:

$$\mathbf{\Omega} \,.\, \boldsymbol{\nabla} I_\nu(\boldsymbol{x}, \mathbf{\Omega}) \quad = \quad E_\nu \, - \, \sigma_\nu \, I_\nu(\boldsymbol{x}, \mathbf{\Omega})$$

- Radiative properties can vary rapidly with frequency.

- Line-by-line (LBL) approach entails computing intensities for individual frequencies followed by integration in frequency space to obtain total quantities:

$$I(\boldsymbol{x}, \mathbf{\Omega}) \quad = \quad \int_{\nu_{\min}}^{\nu_{\max}} I_\nu \, d\nu$$

- This approach, although exceedingly accurate, is impractical for online radiation calculations on complex 3D systems.

- Reduced-order models imperative for reducing cost of evaluating properties (E_ν, σ_ν) and then solving RTEs.

Spectral Reduced-order Models

- **First Step:** Methodology for creating reduced-order groups for which RTEs are solved (not large number of original frequencies):
  - Multi-band Multi-bin based on Planck averaging (Rosseland mean).
  - Method of homogenization.
  - Correlated / Scaled k-distributions

- The last two methods rely on statistics (not assumed spectral distributions) and are said to work more reliably for a broader set of physical situations.

- **Second Step:** Investigate physical criteria and subsequent grouping strategy for identifying which LBL frequencies need to be clustered together (analogous to work on StS kinetics).

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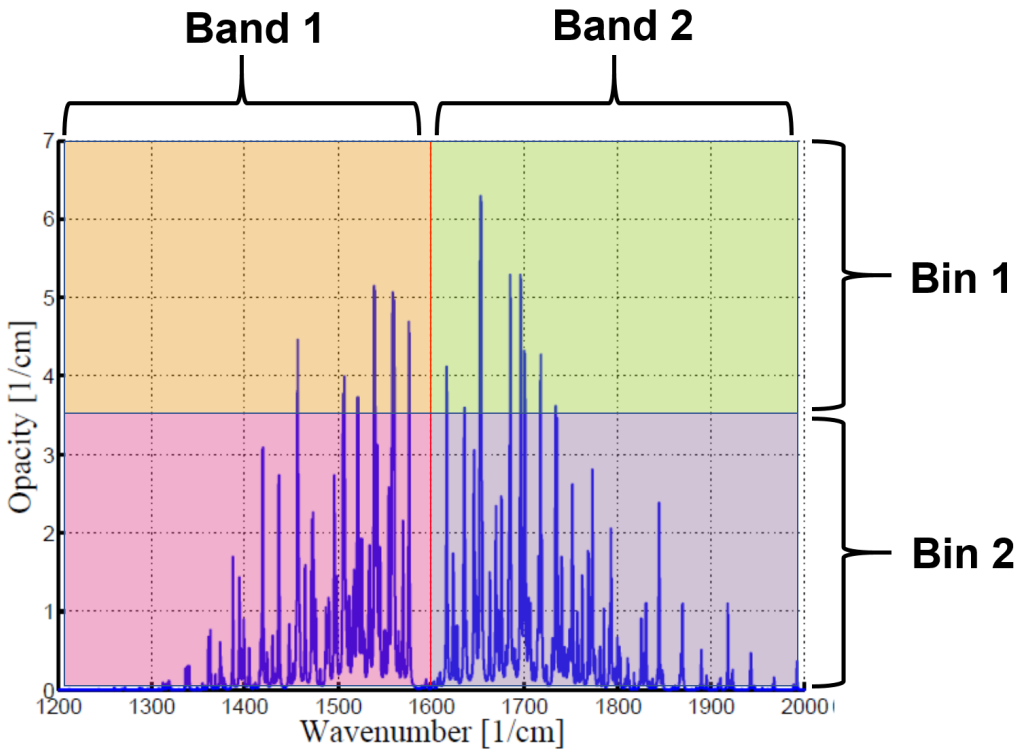
[1] Sahai *et al.*, *Adaptive coarse graining method for energy transfer and dissociation kinetics of polyatomic species*, J. Chem. Phys. (2017).

General Methodology for Spectral Reduced-order Models



Bands based on frequency and bins based on opacity

- Model-reduction techniques differ in what “average” properties are prescribed for groups (band/bin combination).
- More sophisticated clustering approaches expected to change this simple frequency – opacity (continuous interval) grouping paradigm.

Multi-band Multi-bin using Planck Averaging

- This approach assumes a frequency-wise intensity distribution while computing the representative $\hat{\sigma}$ for given group i:

$$\hat{\sigma}_i \;=\; \int \sigma_\nu \, I_\nu \, d\nu \Big/ \int I_\nu \, d\nu$$

- Setting I_ν equal to Planck distribution $B_\nu(T)$ ensures that spectral radiance within a group maximizes entropy (analogous to Boltzmann distribution within chemical bins).
- The maximum entropy formulation becomes more consistent if assumed spectral radiance satisfies constraint based on total group intensity $\hat{I}_i$:

$$\hat{I}_i \;=\; \int I_\nu \, d\nu \;=\; \int B_\nu(T_{rad}) \, d\nu$$

- Re-computing T_{rad} ($\neq T_{flow}$) ensures that integral of Planck weights for spectral averaging matches group intensity.

Theory of Homogenization (Haut *et al.*, JQSRT, 2017)

- Homogenization discards assumed spectral distributions in favor of statistics to derive "averaged" $\hat{\sigma}_i$.
- The method relies on estimating the probability distribution $p(\sigma_\nu)$ (Young measure) of the value of the absorption coefficient $\sigma_\nu(\underline{\phi}_0)$.

$$I_\nu^{exact} = \int_0^\infty I(\sigma_\nu)\, p(\sigma_\nu)\, d\sigma_\nu$$

- Young measure is discretized to obtain the conventional multi-band multi-bin reduced-order model. This involves computing p_{ij} which is the probability of:

$$\sigma_j \leq \sigma_\nu < \sigma_{j+1} \quad \forall \quad \nu \in [\nu_i, \nu_{i+1}]$$

- Discretized Young measure p_{ij} is essentially the probability of being in the i^{th} frequency band and j^{th} opacity bin.
- Total intensity is then computed using a weighted average:

$$I_{total} = \sum_i \sum_j p_{ij}\, I_{ij}$$

Reordered k-distribution (Modest *et al.*, JQSRT, 2003)

- Reodered k-distributions strictly applicable to equilibrium radiation (oscillations induced by absorption coefficients).
- Non-equilibrium radiation modeled using $I_\nu^{neq} = E(\nu, \underline{\phi}) \,/\, \sigma(\nu, \underline{\phi})$
- Original ν-dependent RTE reordered in k-space (absorption coefficient values):

$$I_k = \int_0^\infty I_\nu \, \delta(k - \sigma_\nu(\underline{\phi}_0)) \, d\nu$$

- Non-equilibrium emission-weighted probability density function is defined for frequency band i:

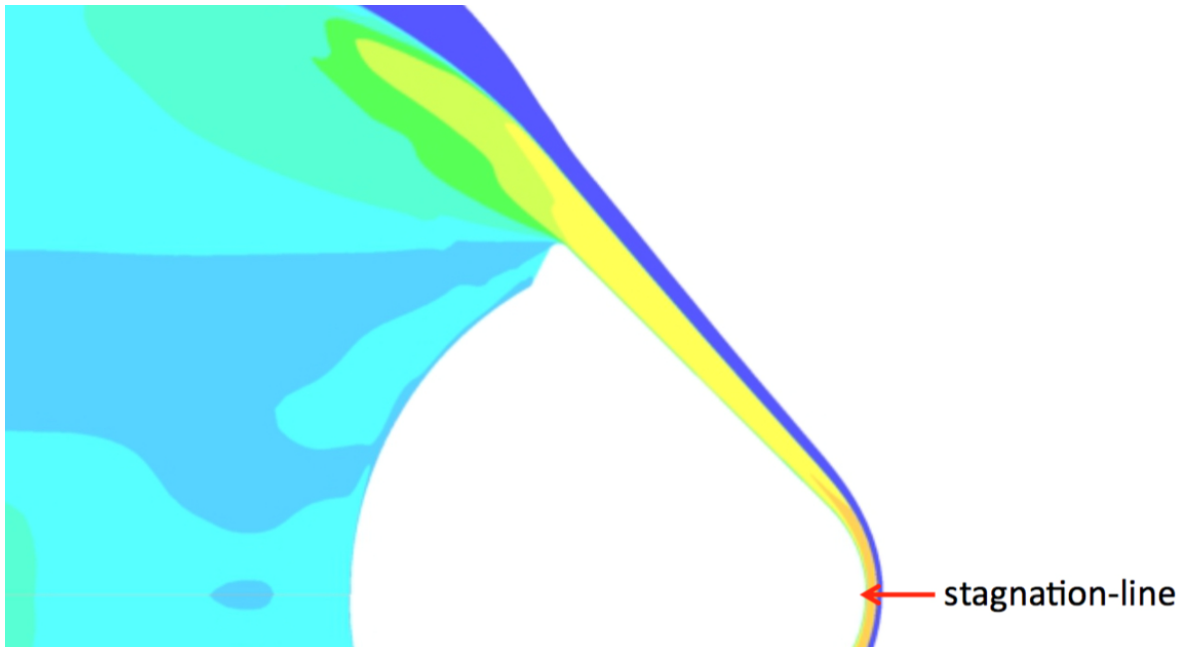
$$f(\underline{\phi}, \underline{\phi}_0, k) = \left[\int_0^\infty I_\nu^{neq}(\underline{\phi}) \, \delta(k - \sigma_\nu(\underline{\phi}_0)) \, d\nu \right] \Big/ \, I_i^{neq}(\underline{\phi})$$

- RTE in the k-space:

$$\boldsymbol{\Omega} \,.\, \boldsymbol{\nabla} I_k = k^*(\underline{\phi}, k) \, f(\underline{\phi}, \underline{\phi}_0, k) \, I_i^{neq}(\underline{\phi}) - k^*(\underline{\phi}, k) \, I_k$$

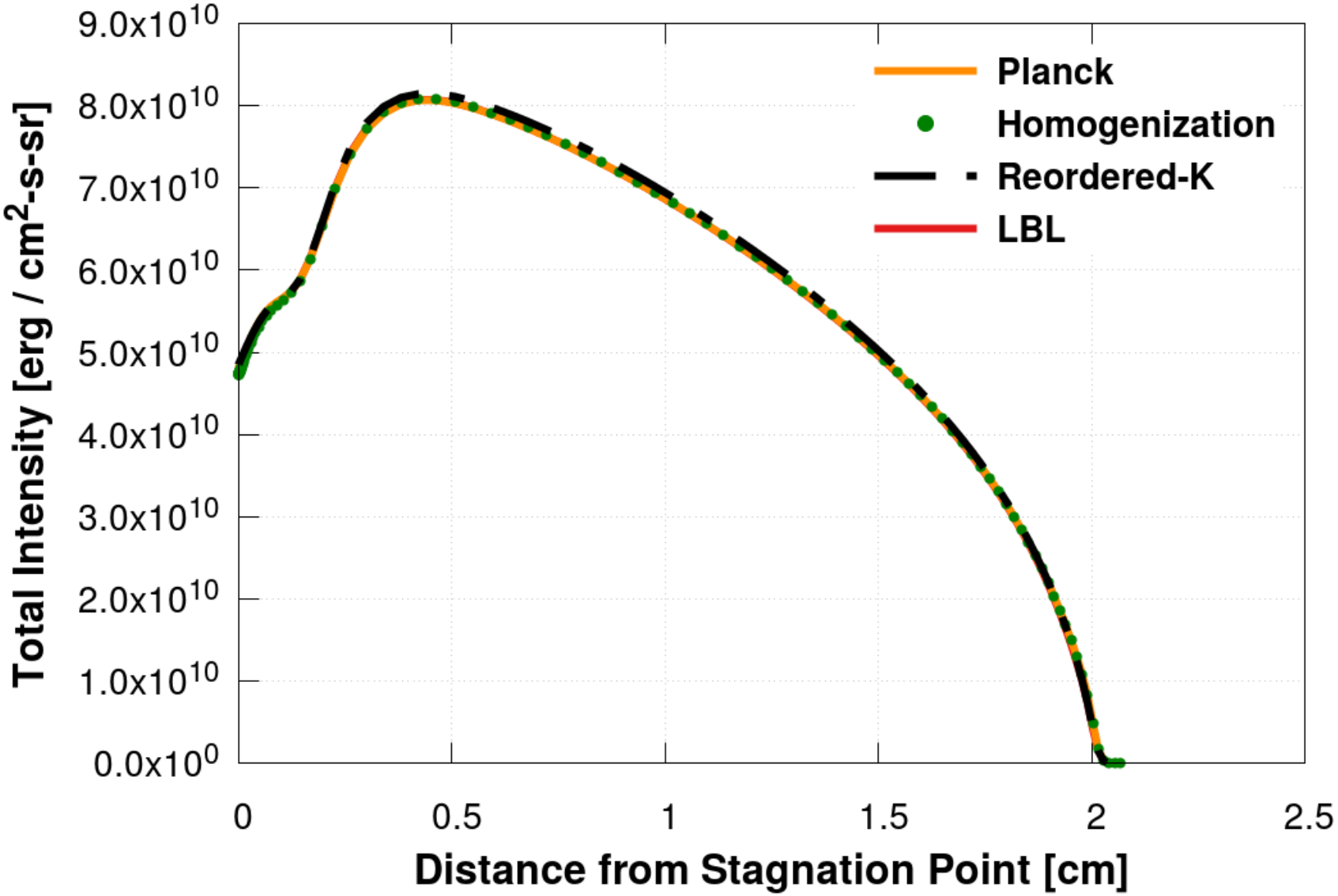
Galileo

- Jupiter entry with ablation products, peak heating point:
  - $U_\infty = 41.6\ km/s$
  - $\rho_\infty = 3.49 \times 10^{-4}\ kg/m^3$
- Strong atomic H lines and atomic continuum from H provide dominant emission from the inviscid region.
- C3 and C2H, and H2 molecular band systems provide boundary layer absorption.
- Original LBL calculations require $\sim \mathcal{O}(10^6)$ frequencies.



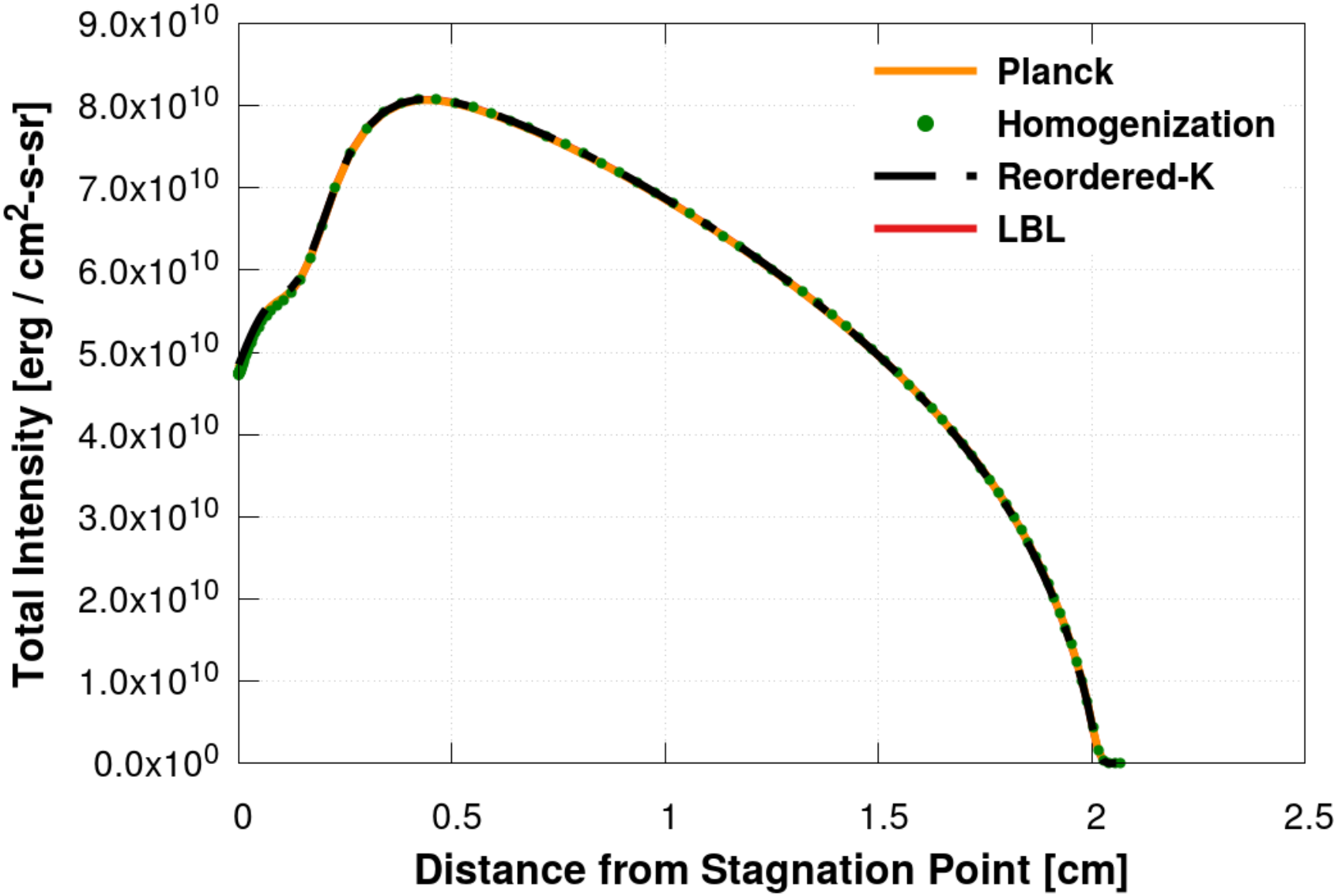
Galileo

- Reduced-order models based on 25 bands $\times$ 25 bins.



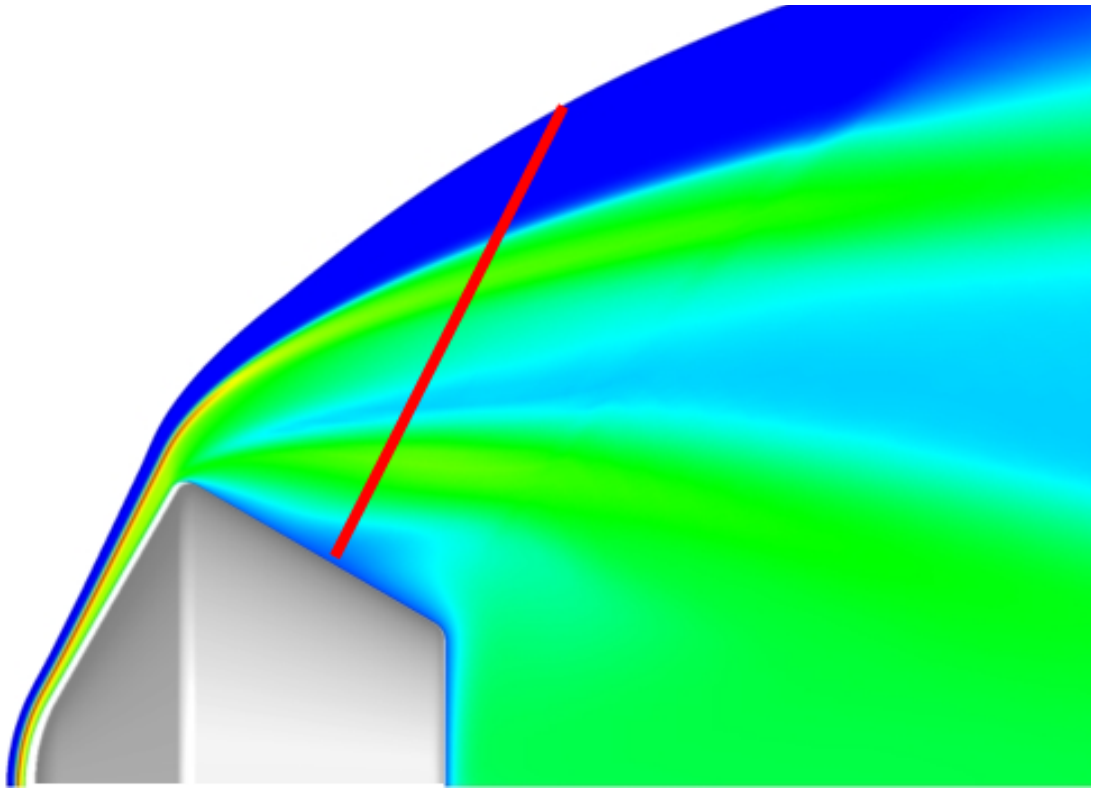
Galileo

- Reduced-order models based on 25 bands $\times$ 50 bins.



Stardust

- Earth entry:
  - $U_\infty = 11.69\ km/s$
  - $\rho_\infty = 1.05 \times 10^{-4}\ kg/m^3$
- Atomic N lines are the dominant contributors.
- Molecular bands and the atomic continuum are also included.
- Original LBL calculations require $\sim \mathcal{O}(10^6)$ frequencies.



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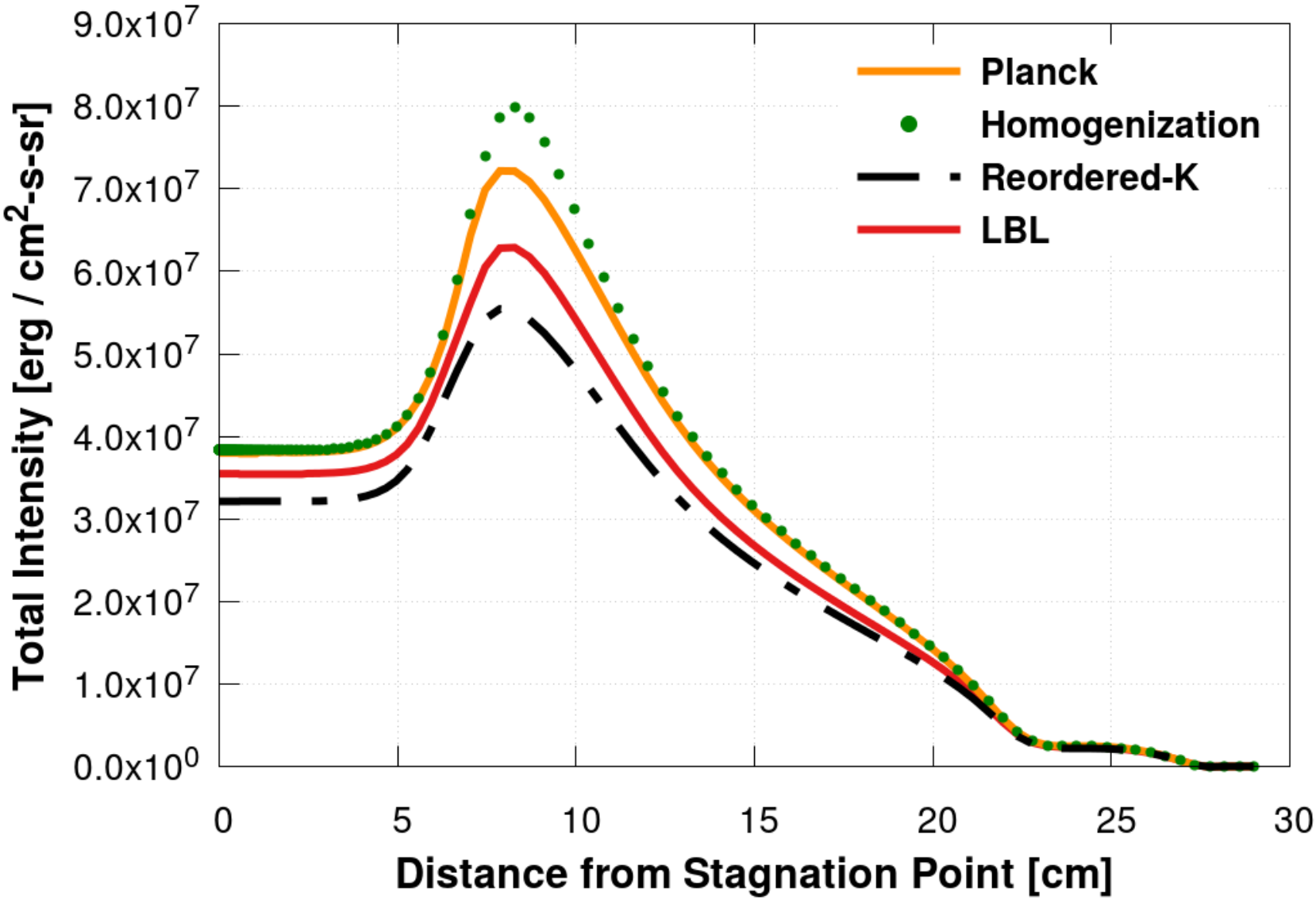

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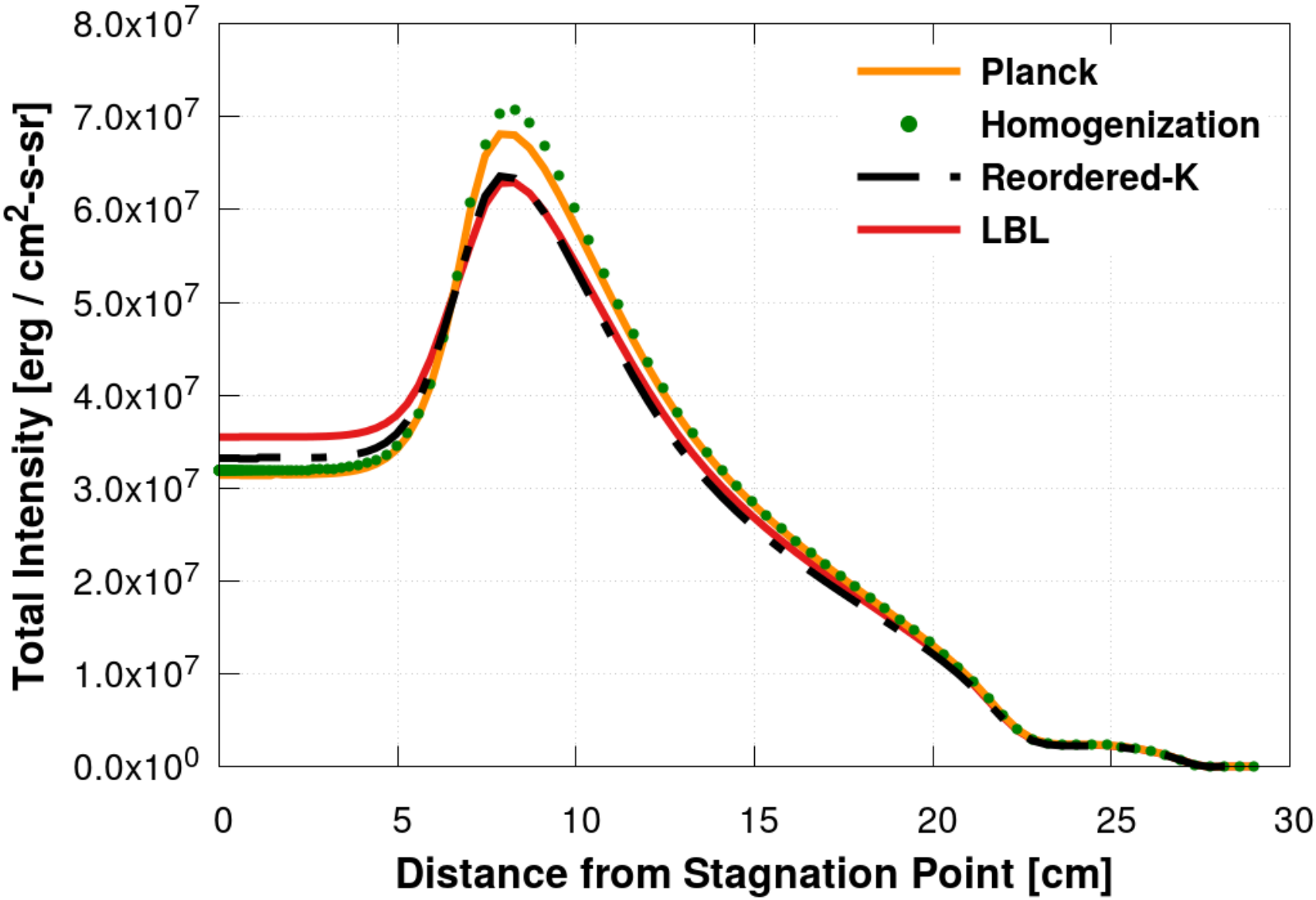
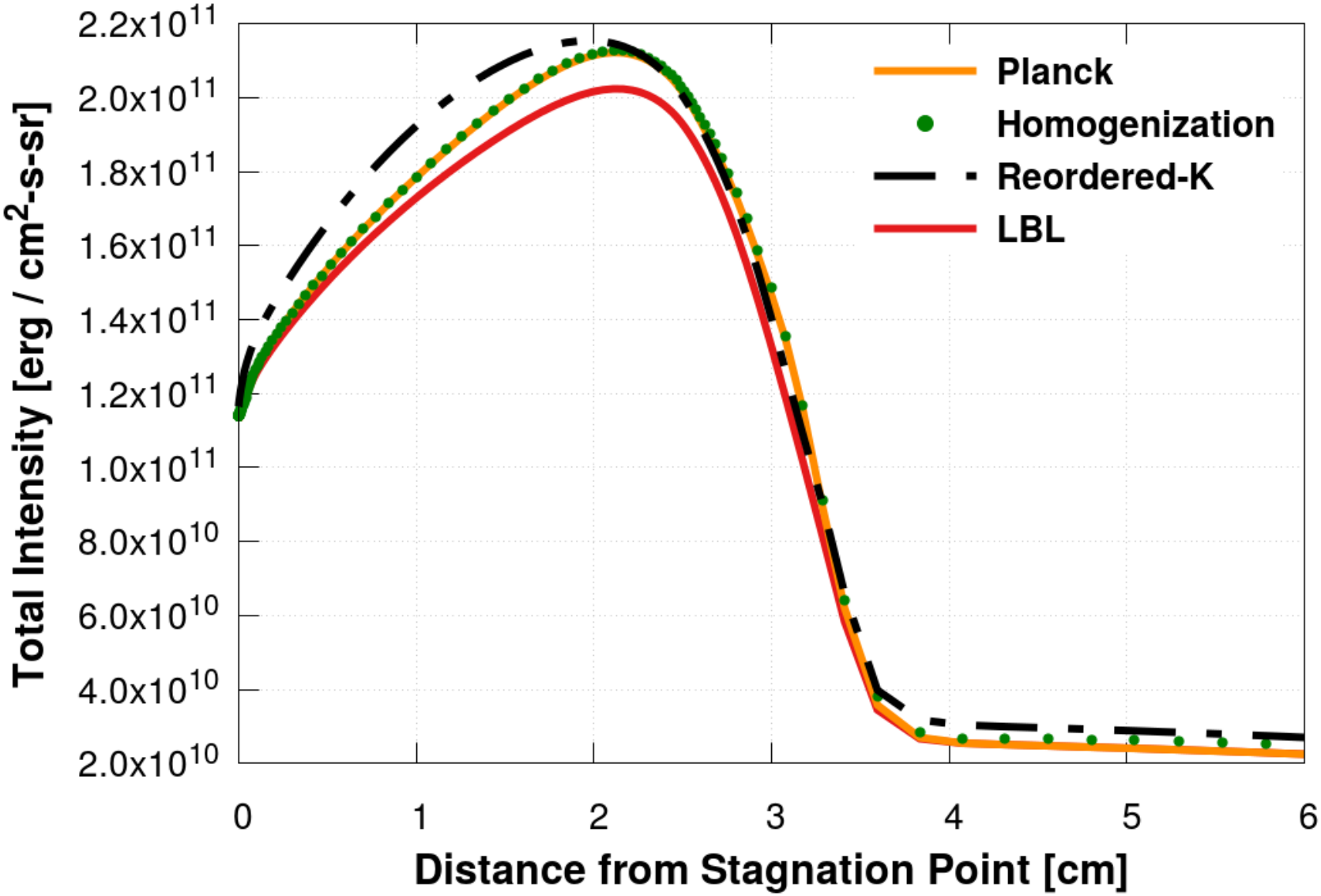


Meteor Precursor

- Earth entry, no ablation products:
  - $U_\infty = 20\ km/s$
  - $\rho_\infty = 9.78 \times 10^{-4}\ kg/m^3$
- Strong N and O lines dominate.
- Original LBL calculations require $\sim \mathcal{O}(10^6)$ frequencies.
- LOS located along the stagnation line

Meteor Precursor

- Reduced-order models based on 25 bands $\times$ 25 bins.



Meteor Precursor

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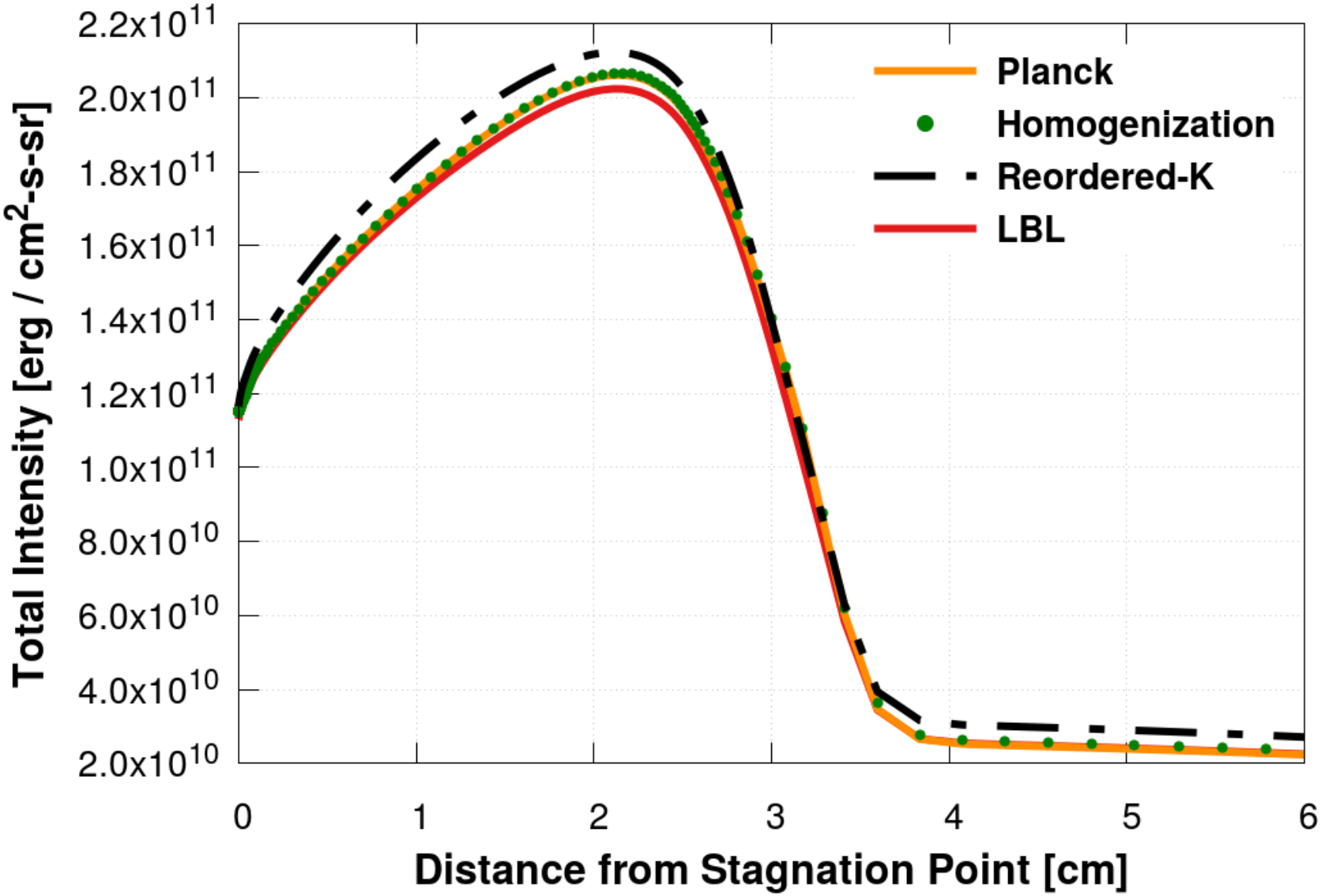

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Radiation Binning Strategy for MBOB Framework

- Grouping criteria for radiation not straightforward (unlike state-to-state chemistry) because spectral intensities uncoupled.
- Conventional grouping focuses on frequency bands + opacity bins.
- Non-intuitive grouping criteria can be evolved by comparing LBL and reduced-order LOS solutions:

$$\begin{aligned} I_\nu(s) &= \cancel{I_\nu(0)\exp\left(-\int_0^s \sigma_\nu\, ds'\right)}^{\;0} \\ &+ \int_0^s E_\nu \exp\left(-\int_{s'}^s \sigma_\nu\, ds''\right)\, ds \end{aligned}$$

- Reduced-order group intensity ($I_{ij} = \int I_\nu d\nu$) is unpacked to obtain frequency-wise intensity:

$$I_\upsilon \approx I_{ij}\,\frac{B_\nu}{\int B_\nu\, d\nu}$$

Radiation Binning Strategy for MBOB Framework

- Medium assumed to be homogeneous in order to simplify analysis.

$$\frac{B_\nu}{\int B_\nu \, d\nu} E_{ij} \exp\left(-\int_{s'}^{s} \sigma_{ij} \, ds''\right) = E_\nu \exp\left(-\int_{s'}^{s} \sigma_\nu \, ds''\right)$$

- Term-by-term comparison of the Taylor series expansion allows group and spectral properties to be compared:

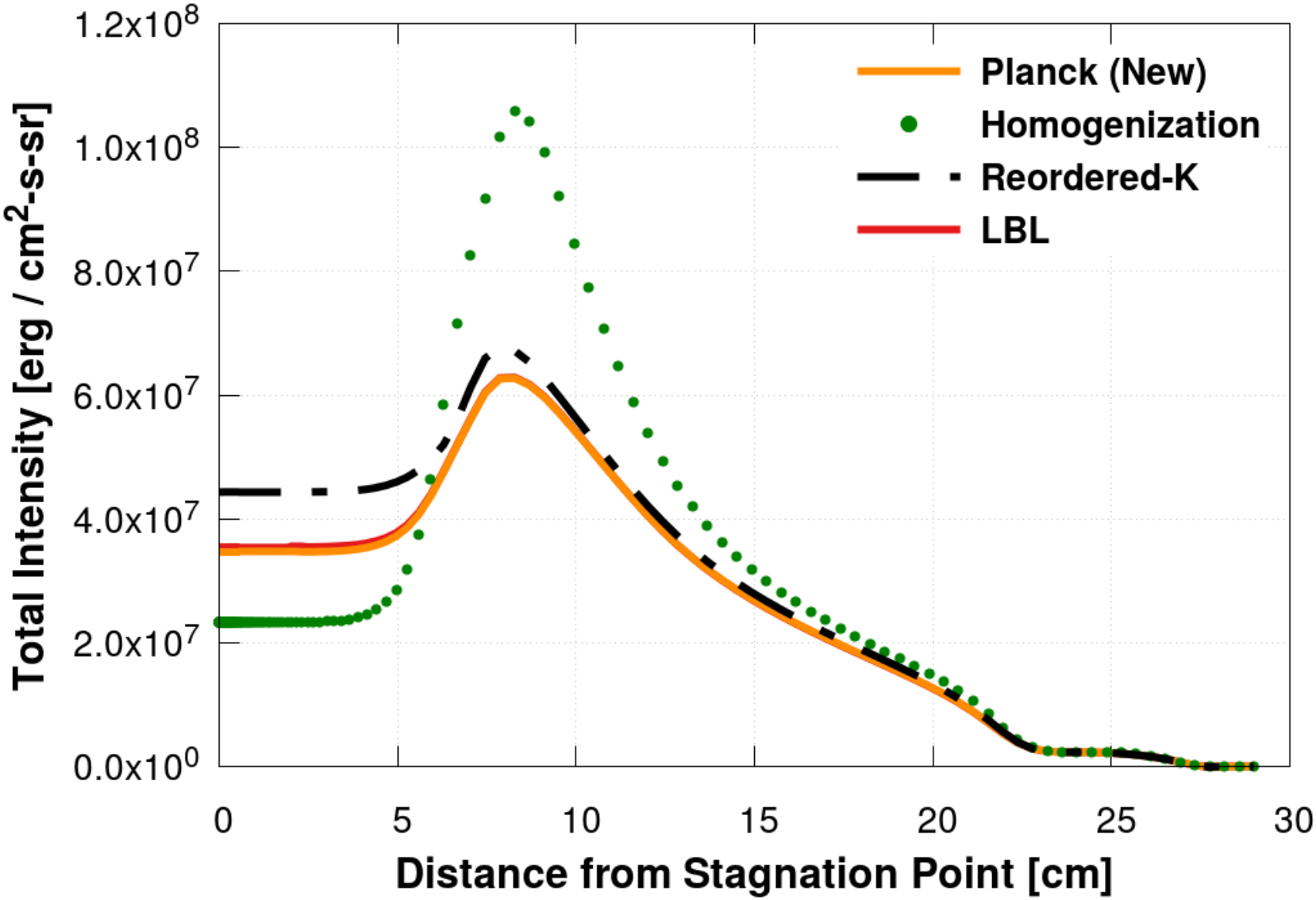
$$E_{ij} \, \sigma_{ij}^n \frac{B_\nu}{\int B_\nu \, d\nu} = E_\nu \sigma_\nu^n$$

$$\Rightarrow \frac{E_\nu}{E_{ij}} = \frac{E_\nu \, \sigma_\nu}{E_{ij} \, \sigma_{ij}} = \frac{E_\nu \, \sigma_\nu^2}{E_{ij} \, \sigma_{ij}^2} = \ldots = \text{Constant}$$

- $\sigma_\nu = \sigma_{ij} = \text{Constant}$ is a trivial solution – rationale for regular opacity binning.
- Generalized approach – bands based on E_ν and bins based on $E_\nu \, \sigma_\nu$.

Stardust

- Reduced-order models based on 20 bands $\times$ 20 bins.



Stardust

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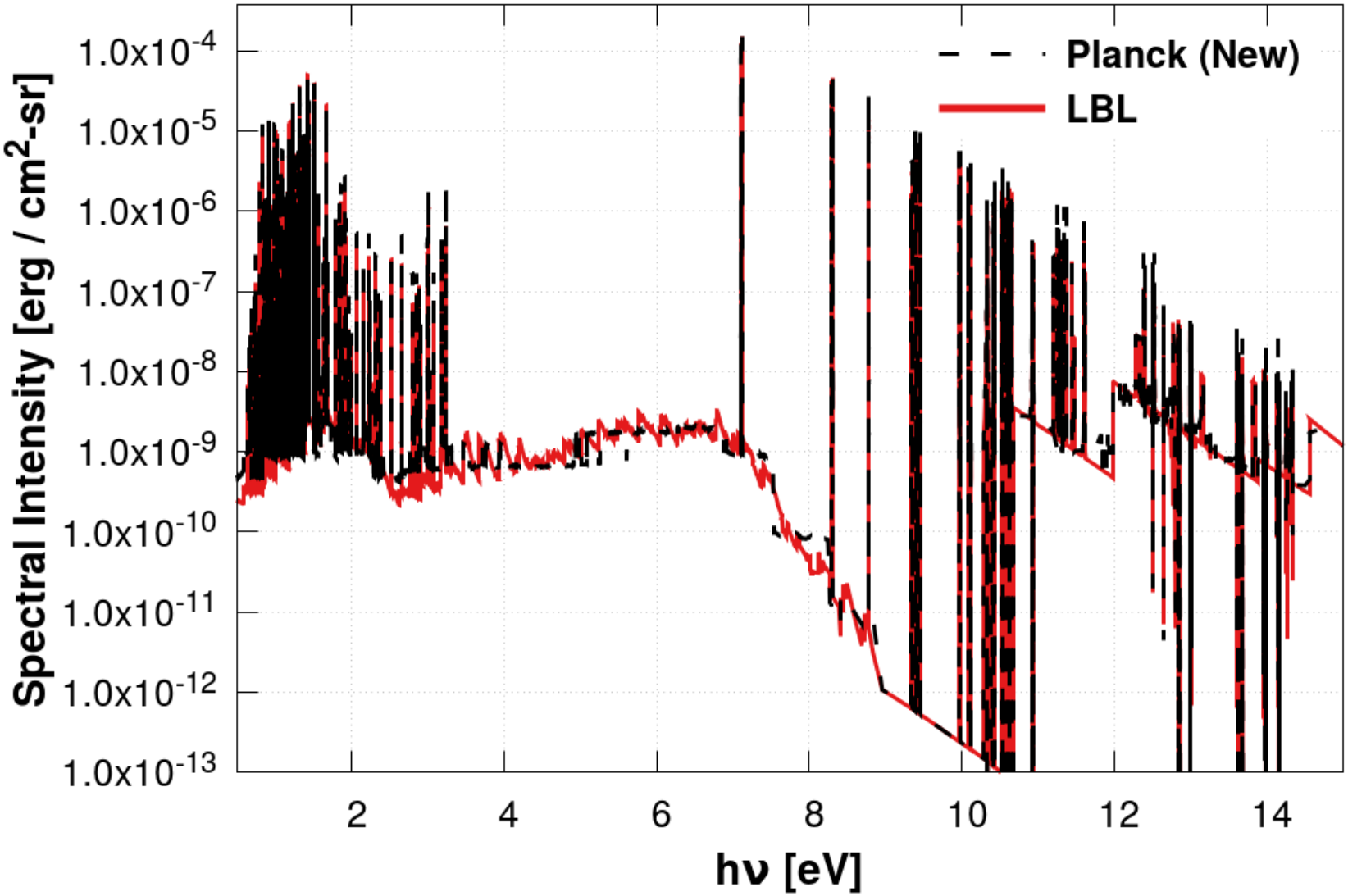

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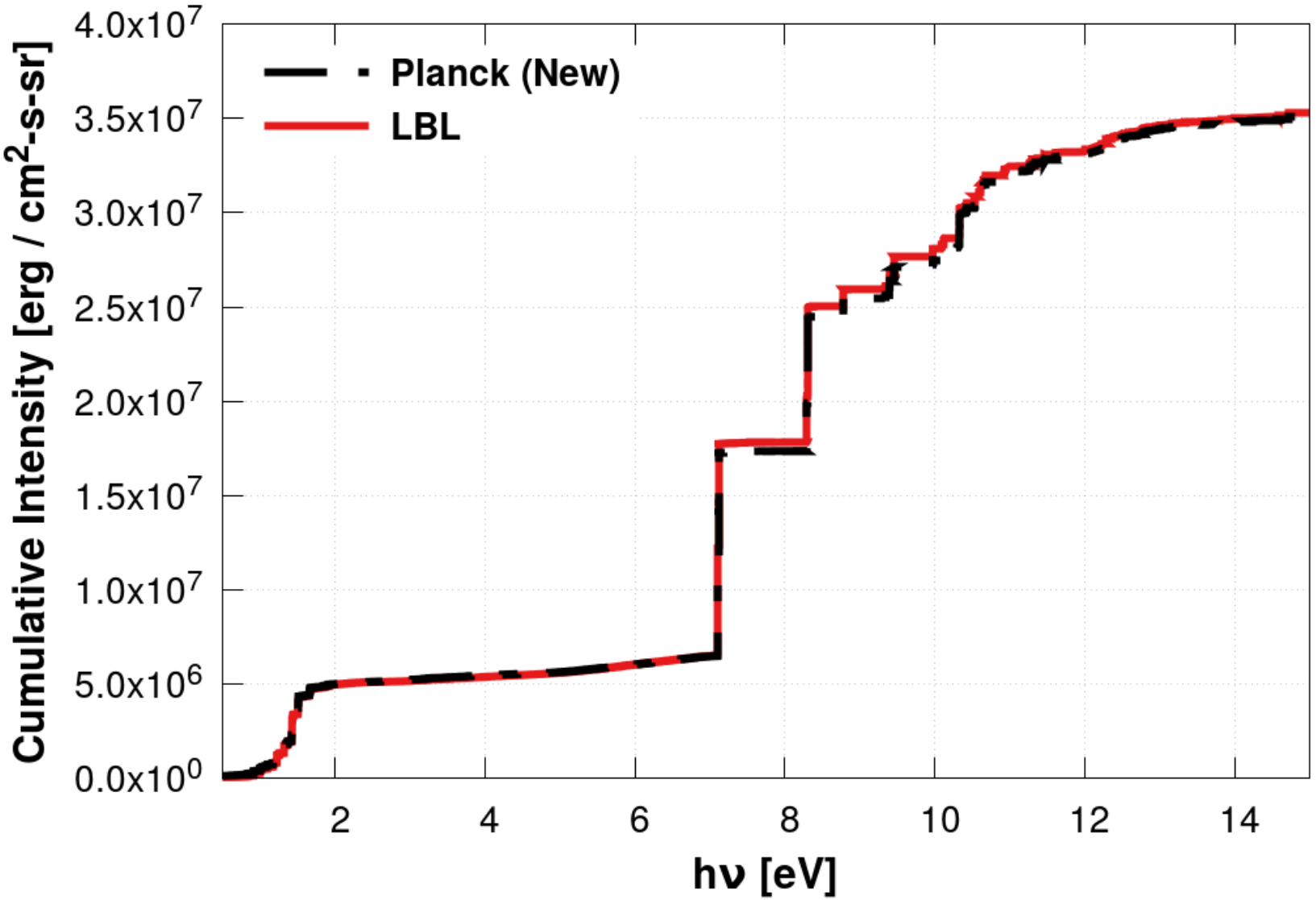
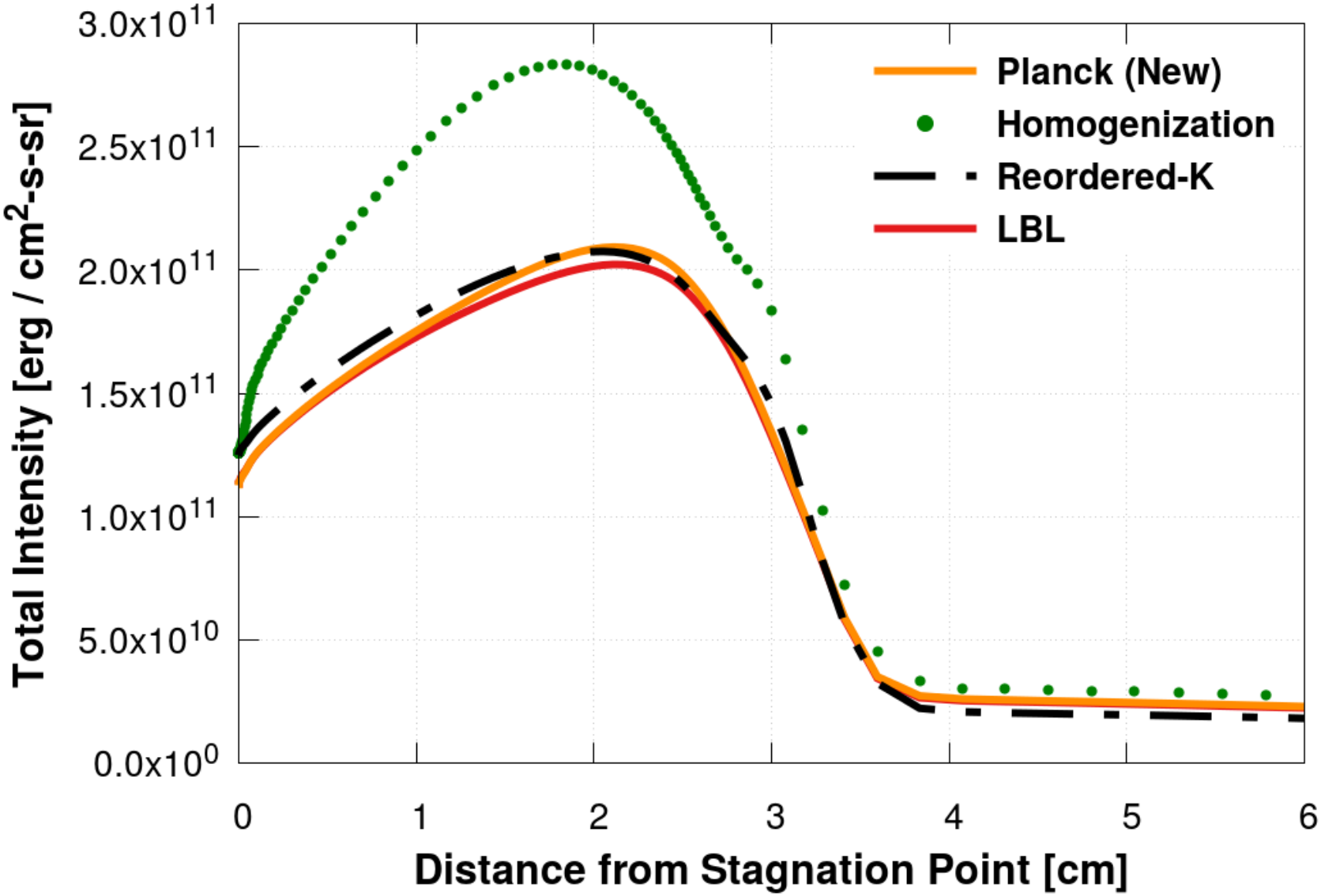


Meteor

- Reduced-order models based on 10 bands $\times$ 10 bins.



Meteor

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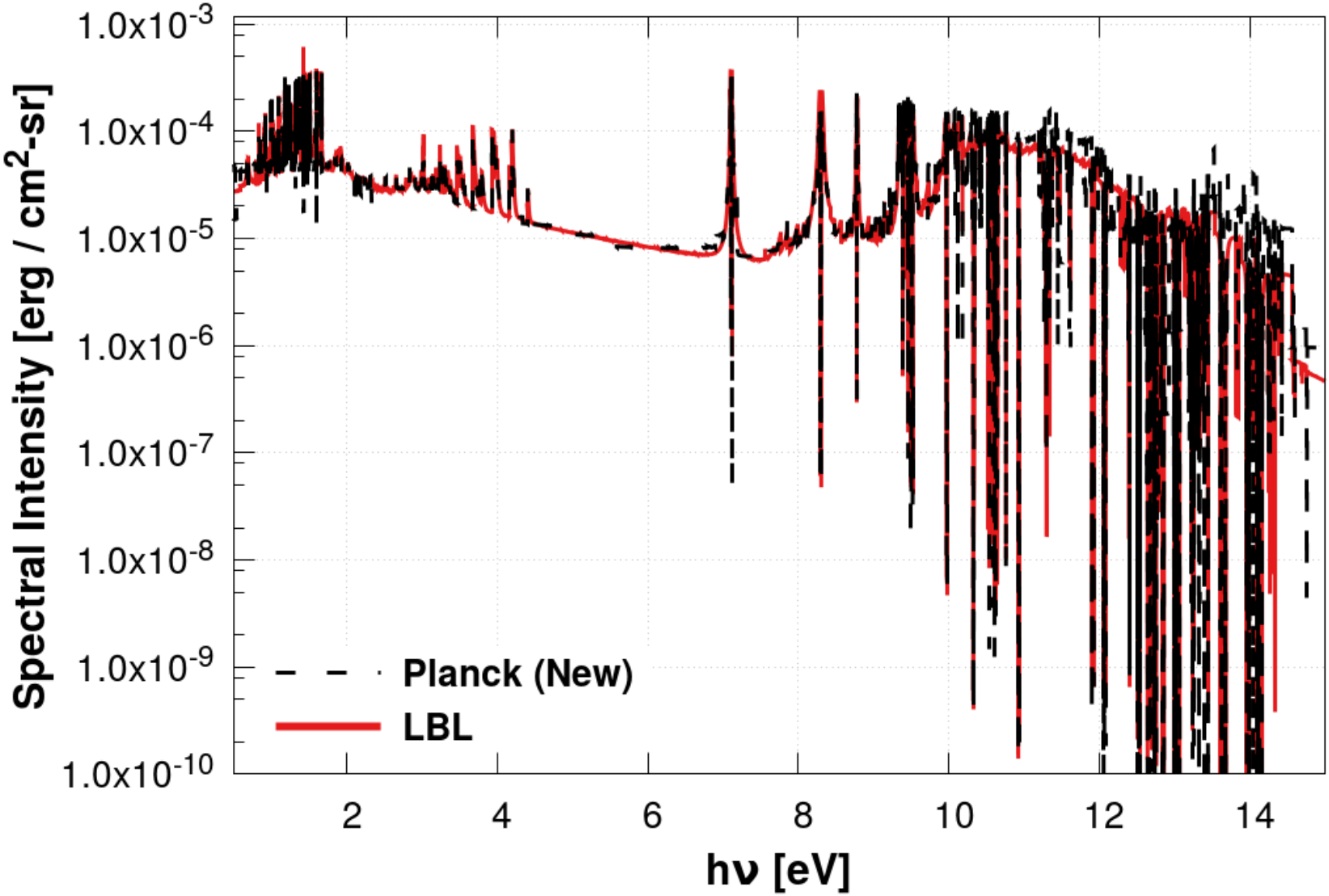

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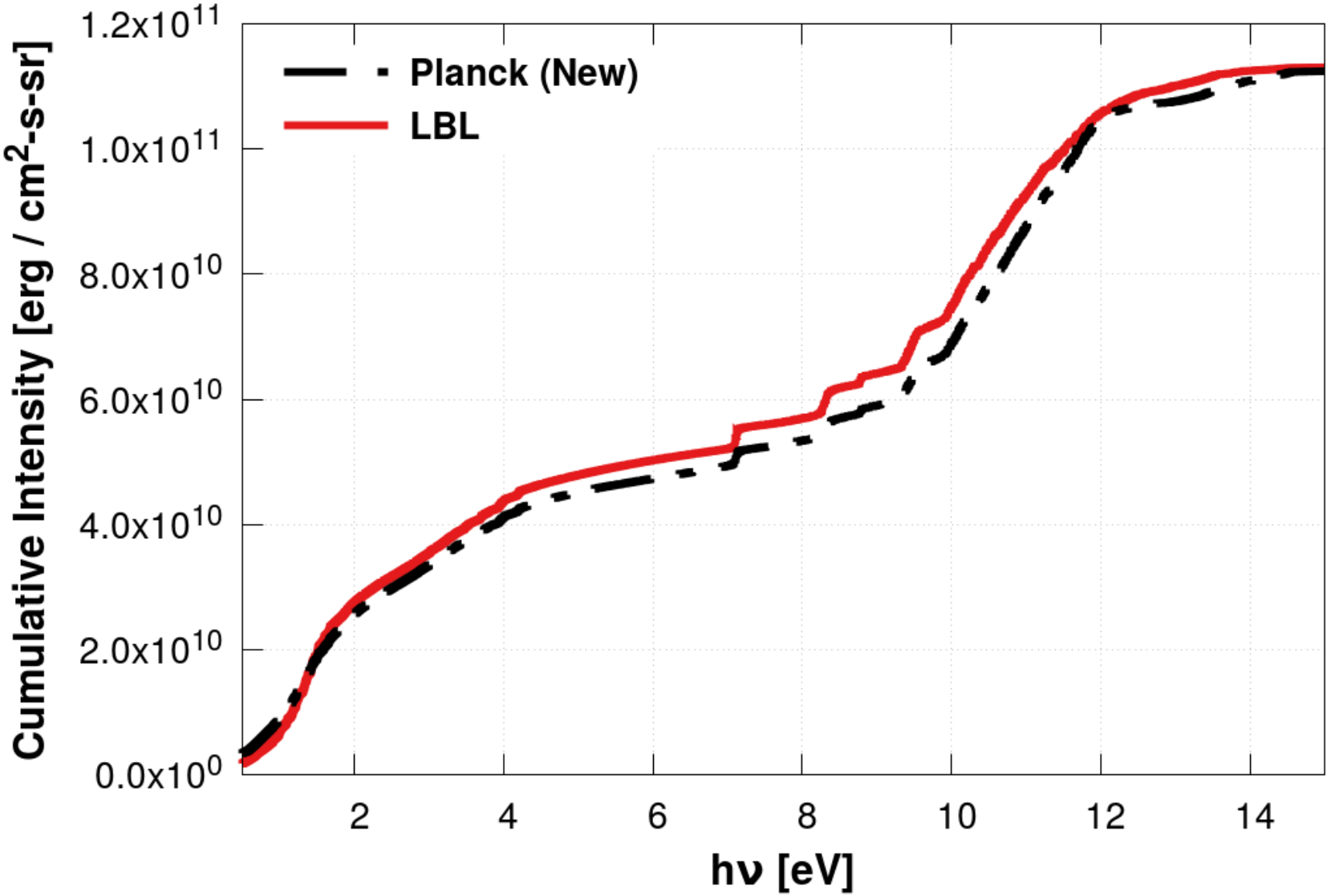

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Coupled Radiation-Flow Solutions for 3D Meshes

- Efficient spectral reduced-order models and RTE solution methodology key for managing computational loads.
- Angular integration performed with focus on reducing the number of rays required for accurate solution.
- Total radiative heat flux (and its divergence) computed using a Gaussian / Lebedev type angular quadrature:

$$\mathbf{q}^{rad} = \int_{4\pi} I_\nu \, \mathbf{\Omega} \, d\mathbf{\Omega} = \sum_m w^m \, I_\nu^m \, \mathbf{\Omega}^m$$

- FEM / FVM based discretization avoids concomitant challenges associated with ray tracing.
- Angularly / spatially resolved radiation allows species continuity source terms to be computed while accounting for non-local absorption.

Finite Volume based RTE Solver

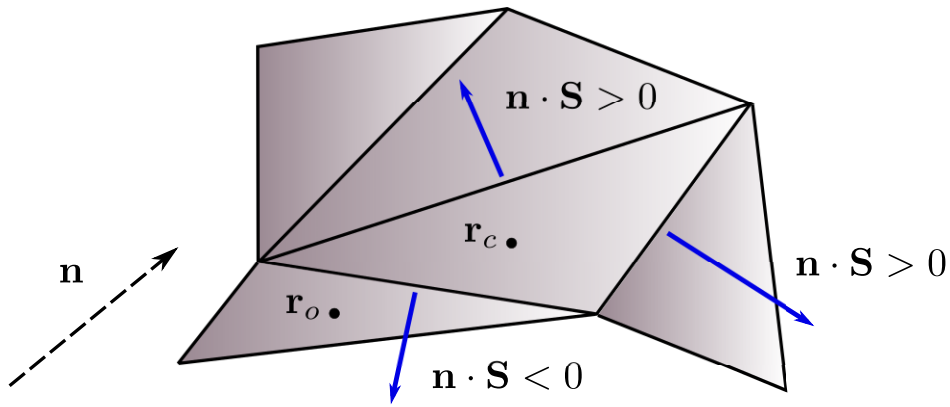
- A finite-volume formulation is obtained by integrating the RTE in direction $\mathbf{n}$ over an element (and then discretizing it):

$$\sum_f \mathbf{n} \,.\, \mathbf{S}^f \, I_\nu^f \;=\; -\hat{\sigma}_\nu \, I_\nu^e \, V_e$$

- Flux summation is evaluated by first-order upwinding:

$$I_\nu^f = \begin{cases} I_\nu^e \,, & \text{for } \mathbf{n} \,.\, \mathbf{S}^f > 0 \\ I_\nu^{neigh} \,, & \text{for } \mathbf{n} \,.\, \mathbf{S}^f < 0 \end{cases}$$

$$I(\mathbf{r}_c) = -\frac{\sum\limits_{\mathbf{n} \,.\, \mathbf{S} < 0} \mathbf{n} \,.\, \mathbf{S} \, I(\mathbf{r}_o)}{\sum\limits_{\mathbf{n} \,.\, \mathbf{S} > 0} \mathbf{n} \,.\, \mathbf{S} + \sigma(\mathbf{r}_c) \, \Omega_c}$$



- Sparse linear system re-ordered into lower triangular system by **sweeping the mesh** according to an **advance-order list**.

Self-consistent Radiation-flow Coupling

- Two-way coupling – Flowfield solution passed on to radiation solver while radiative field information (source terms) provided to flow solver.
- Rate constants for radiative processes involving emission and absorption (no escape factor assumption) between species l and u are:

$$\bar{K}^{em}_{u,l} = \frac{\mathcal{M}_u}{\rho_u N_A} \int E^{u,l}_{\nu} \, d\nu$$

$$K^{ab}_{l,u} = \frac{\mathcal{M}_l}{\rho_l N_A} \int \left(\sigma^{l,u}_{\nu} \oint_{4\pi} I_{\nu} d\mathbf{\Omega} \right) d\nu$$

- Source terms for species continuity and energy equations:

$$\dot{\omega}^{rad}_l = \sum_{\forall u | u \neq l} \left(-K^{ab}_{l,u} \, \rho_l + \bar{K}^{em}_{u,l} \, \rho_u \right)$$

$$\Omega^{rad} = -\boldsymbol{\nabla} \cdot \mathbf{q}^{rad} = -\boldsymbol{\nabla} \cdot \int \oint_{4\pi} I_{\nu} \, \mathbf{\Omega} \, d\mathbf{\Omega} \, d\nu$$

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Mars 2020 3D Wake Flows: $\mathrm{CO_2} - \mathrm{M}$ StS Model

- $\mathbf{9,056}$ **vibrational levels** for ground electronic state of CO_2.
- Each level defined using 4 modes: 1 symmetric stretching, 2 degenerate bending, and 1 asymmetric stretching.
- CO_2 molecule has multiple pathways for vibrational relaxation ($\sim \mathbf{100,000}$ **possible transitions** in current model):

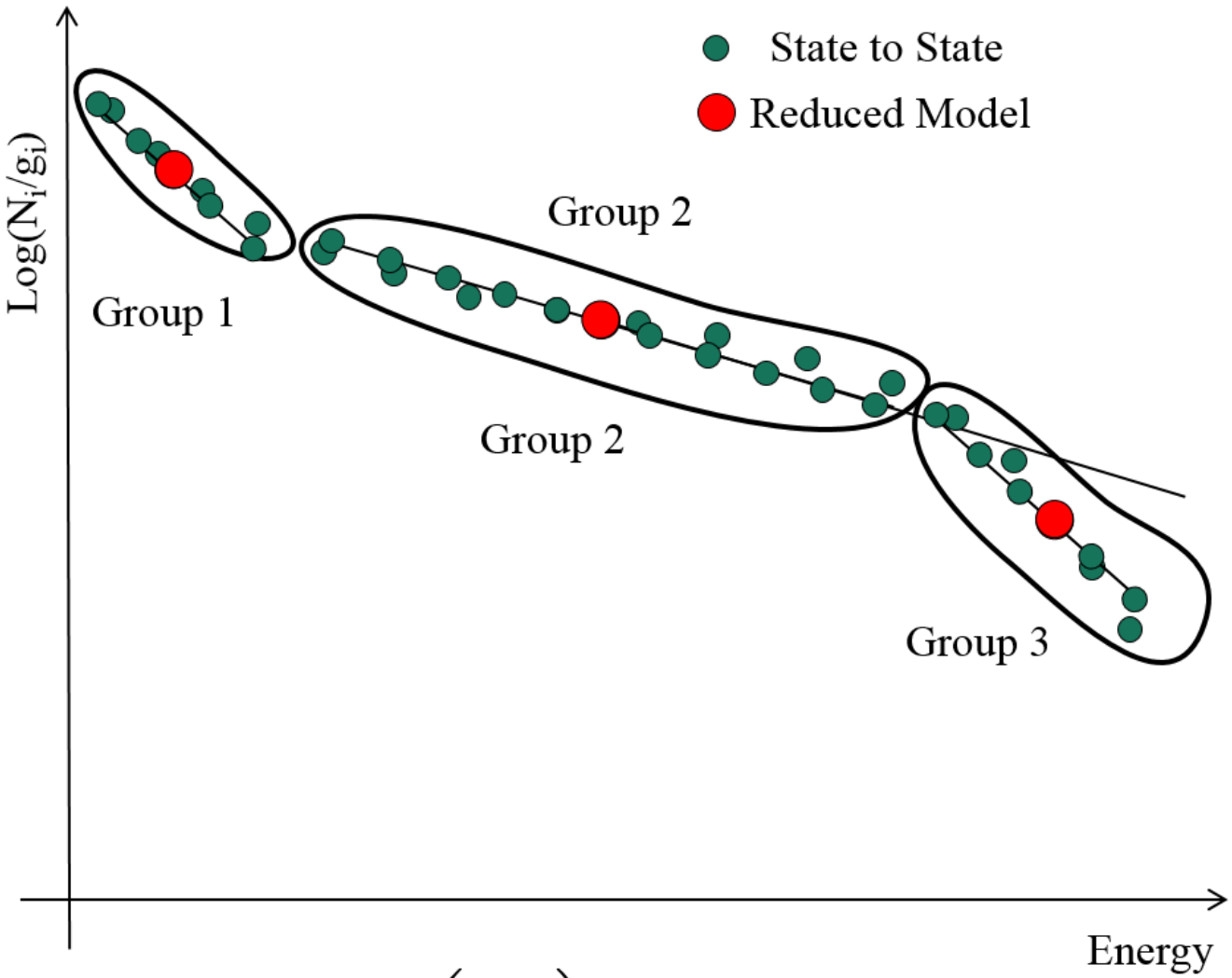
$$
\begin{aligned}
\mathrm{VT}_2 &: \mathrm{CO_2}(v_1, v_2, v_3) + \mathrm{M} \longleftrightarrow \mathrm{CO_2}(v_1, v_2 \pm 1, v_3) + \mathrm{M} \\
\mathrm{VV}_{1-2} &: \mathrm{CO_2}(v_1, v_2, v_3) + \mathrm{M} \longleftrightarrow \mathrm{CO_2}(v_1 \pm 1, v_2 \mp 2, v_3) + \mathrm{M} \\
\mathrm{VV}_{2-3} &: \mathrm{CO_2}(v_1, v_2, v_3) + \mathrm{M} \longleftrightarrow \mathrm{CO_2}(v_1, v_2 \pm 3, v_3 \mp 1) + \mathrm{M} \\
\mathrm{VV}_{1-2-3} &: \mathrm{CO_2}(v_1, v_2, v_3) + \mathrm{M} \longleftrightarrow \mathrm{CO_2}(v_1 \pm 1, v_2 \pm 1, v_3 \mp 1) + \mathrm{M}
\end{aligned}
$$

- Dissociation/recombination occurs as follows:

$$\mathrm{CO_2}(v_1, v_2, v_3) + \mathrm{M} \longleftrightarrow \mathrm{CO} + \mathrm{O} + \mathrm{M}$$

[1] I. Armenise, E.V. Kustova. *State-to-state models for CO_2 molecules: From the theory to an application to hypersonic boundary layers*. Chemical Physics 415 (2013).

Mars 2020 3D Wake Flows: Coarse Grain Method

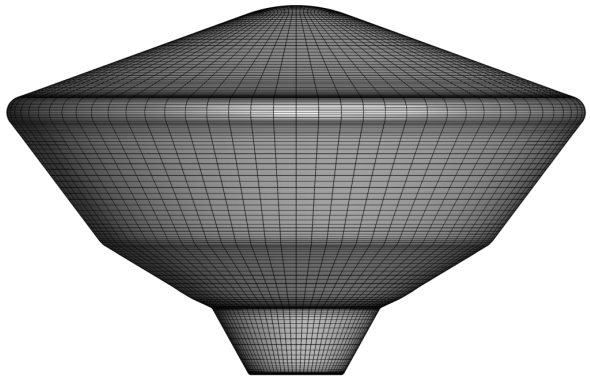


$$\log\left(\frac{g_i}{N_i}\right) = \alpha_g + \beta_g \epsilon_i$$

Mars 2020 3D Wake Flows: Computational Setup

$\mathbf{V}_\infty\ [km/s]$	$\rho_\infty\ [kg/m^3]$	$\mathbf{T}_\infty\ [K]$	$\alpha\ [K]$
5.46	8.44E-5	144	15.26
4.64	1.05E-4	184	15.65
3.89	**1.84E-3**	**193**	**15.88**

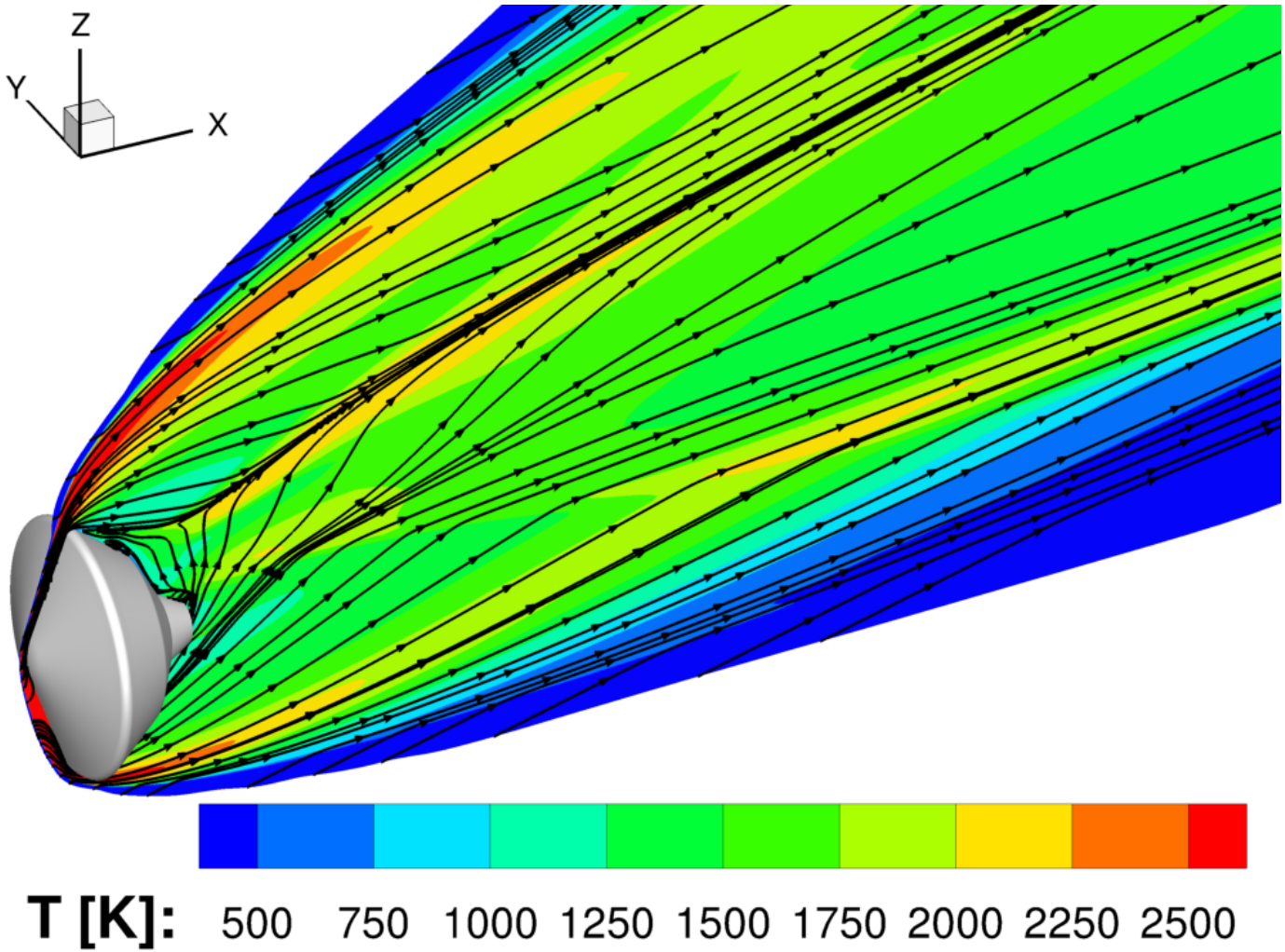
1) Trajectory points considered



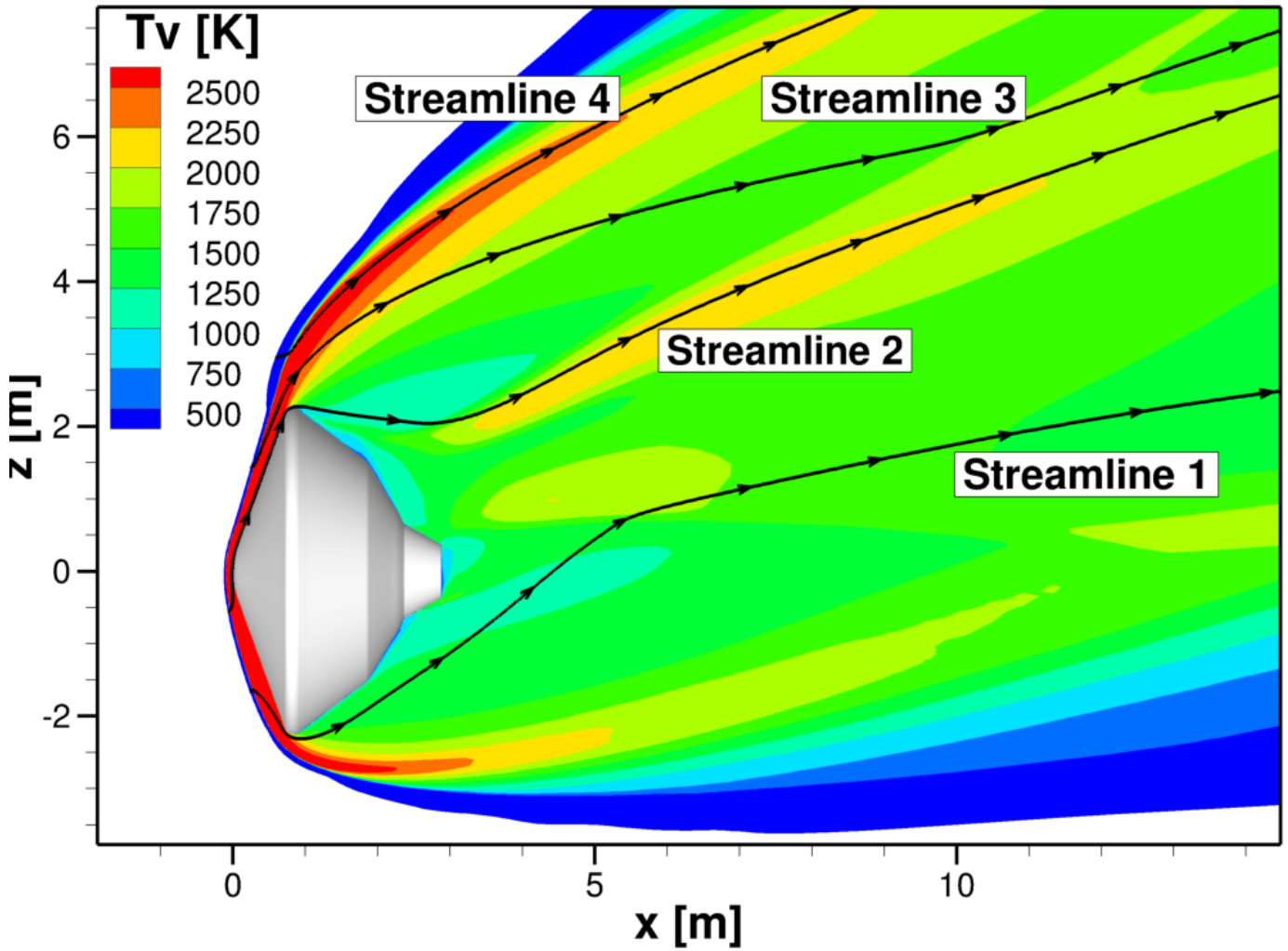
2) Mars 2020 vehicle

- Three-dimensional Mars 2020 mesh with $\sim 2 \times 10^6$ mesh elements and 170 quadrature directions.
- Gas mixture includes: 10 CO_2 Bins, CO, O_2, C, O.
- Compare flowfields (US3D) and resultant IR radiation (NERO) for 1-T / 2-T Boltzmann and reduced-order StS models.
- Radiative transitions in 1.5, 2.7, and 4.5 μm bands are considered.

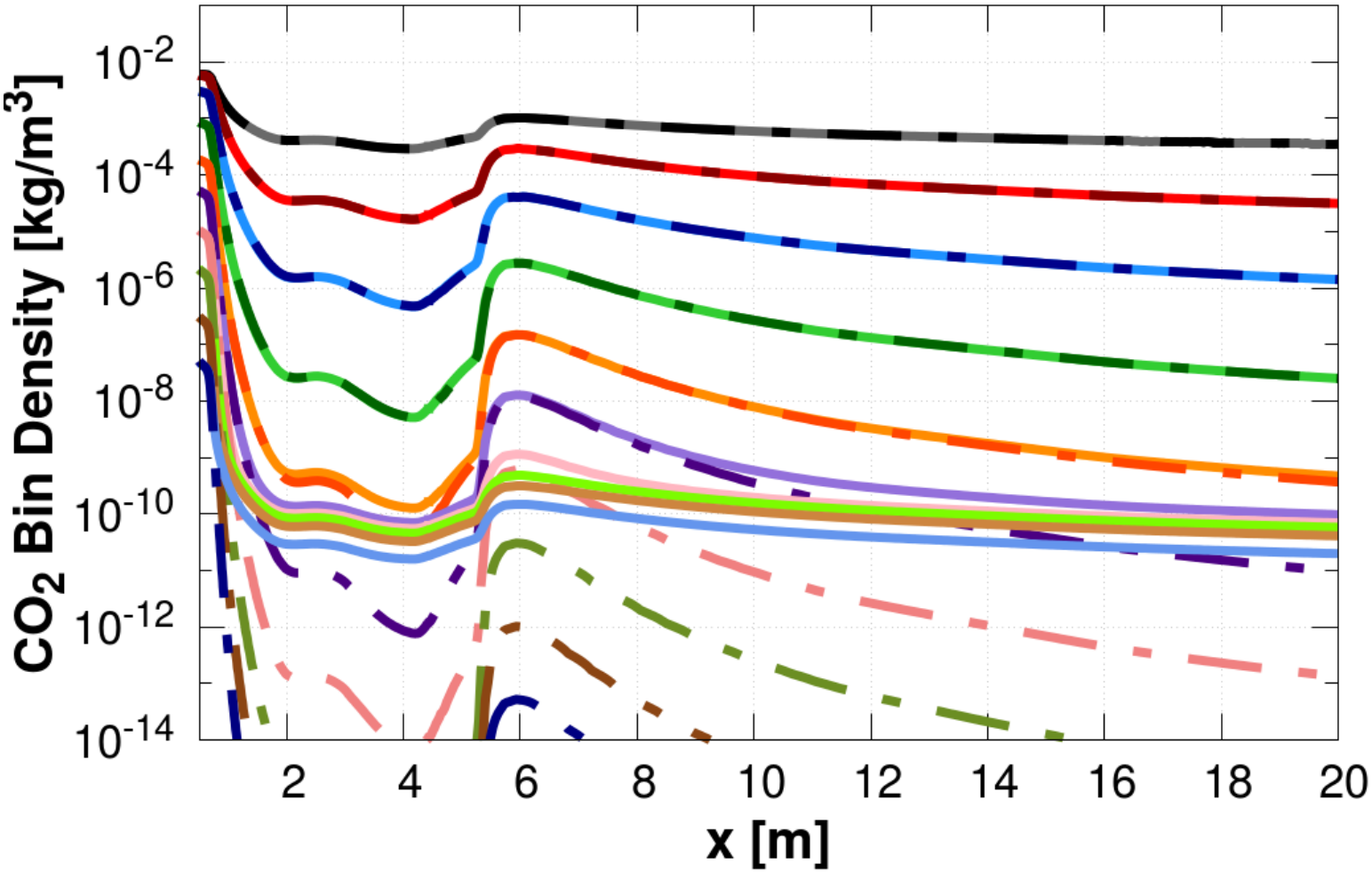
Mars 2020 Wake Flows: $\mathbf{V}_\infty = 3.89\ km/s$



Mars 2020 Wake Flows: $\mathbf{V}_\infty = 3.89\ km/s$

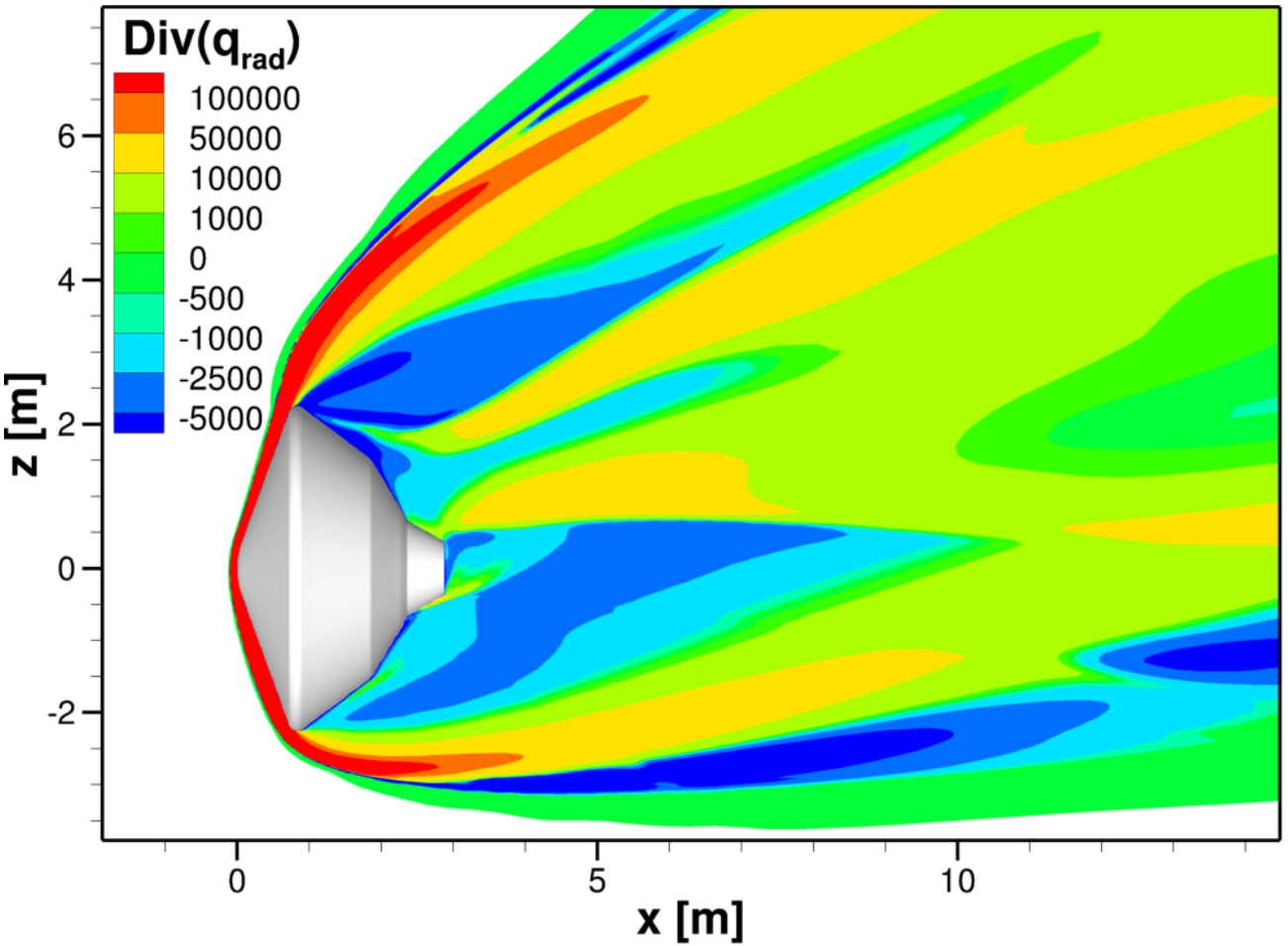


Mars 2020 Wake Flows: $\mathbf{V}_\infty = 3.89\ km/s$



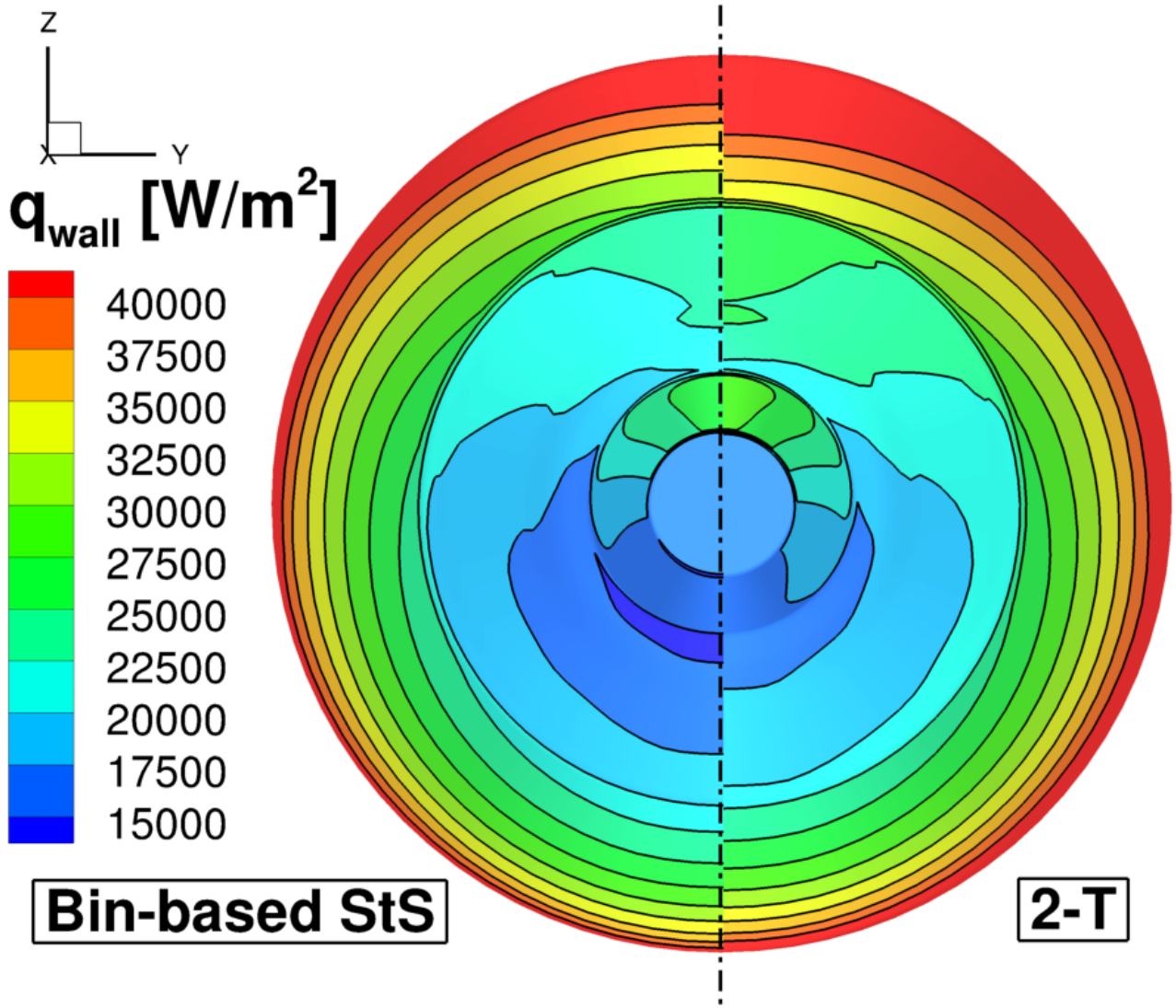
Streamline 2: Solid Lines – Reduced-order StS, Dashed Lines – 2T

Mars 2020 Wake Flows: $\mathbf{V}_\infty = 3.89\ km/s$



$$-\Omega^{rad} = \boldsymbol{\nabla} \cdot \mathbf{q}^{rad} = \boldsymbol{\nabla} \cdot \int \oint_{4\pi} I_\nu \, \boldsymbol{\Omega} \, d\boldsymbol{\Omega} \, d\nu$$

Mars 2020 Wake Flows: $\mathbf{V}_\infty = 3.89\ km/s$



Summary and Future Work

Summary

- MBOB with Planck-averaging just as accurate as statistics-based model reduction methods (that still rely on reordering σ_ν).
- Non-intuitive grouping strategies crucial for improving predictions for total and spectral quantities.
- Efficiency gains through reduced-order spectral models and simpler angular/spatial discretization enable coupled radiation-flow calculations even for complex 3D geometries.
- Complete characterization of CO_2 wake flows using reduced-order thermochemistry bins and self-consistent radiation coupling.

Future Work

- Experiment with other spatial discretization schemes for RTEs.
- Perform flow-radiation coupled calculations for other sytems.

Homogenization: Extension to Non-Equilibrium Radiation

- Original framework developed only for equilibrium radiation with fluctuations induced solely by absorption coefficients.
- Non-equilibrium emission intensity : $I_\nu^{neq} = E(\nu, \underline{\boldsymbol{\phi}}) \,/\, \sigma(\nu, \underline{\boldsymbol{\phi}})$
- Probability distribution computed using weighted integrals (for reference state):

$$p_{ij} = \int\limits_{\nu \in \text{bin } j} I_\nu^{neq}\, d\nu \Bigg/ \int\limits_{\nu \in \text{band } i} I_\nu^{neq}\, d\nu$$

- Bin opacity computed using weighted average:

$$\sigma_{ij} = \int\limits_{\nu \in \text{bin } j} \sigma(\nu, \boldsymbol{T})\, I_\nu^{neq}\, d\nu \Bigg/ \int\limits_{\nu \in \text{bin } j} I_\nu^{neq}\, d\nu = \int\limits_{\nu \in \text{bin } j} E_\nu\, d\nu \Bigg/ \int\limits_{\nu \in \text{bin } j} E_\nu / \sigma_\nu\, d\nu$$

Homgenization: Extension to Non-Equilibrium Radiation

- Bin-wise source term can be computed in manner analogous to equilibrium radiation.
- Tested multiple forms for the source term – most accurate based on conserving total emission:

$$E_{ij} = \int_{\nu \in \text{bin } j} E_\nu \, d\nu \times \left(\frac{\int_{\nu \in \text{band } i} E_\nu / \sigma_\nu \, d\nu}{\int_{\nu \in \text{bin } j} E_\nu / \sigma_\nu \, d\nu} \right)_{\text{Ref}} = \frac{\int_{\nu \in \text{bin } j} E_\nu \, d\nu}{p_{ij}}$$

- σ_{ij} and E_{ij} can be pre-computed for different thermodynamic states.
- Computing total intensities for individual bands requires solving the RTEs for constituent bins (with properties σ_{ij} and E_{ij}) and then averaging using p_{ij} as weights.

Reordered k-distribution

- k-distribution based on f can be ill-behaved, making integration in k space difficult.
- Transformation into smoother g-space performed through division by $f(\underline{\phi_0}, \underline{\phi}_0, k)$:

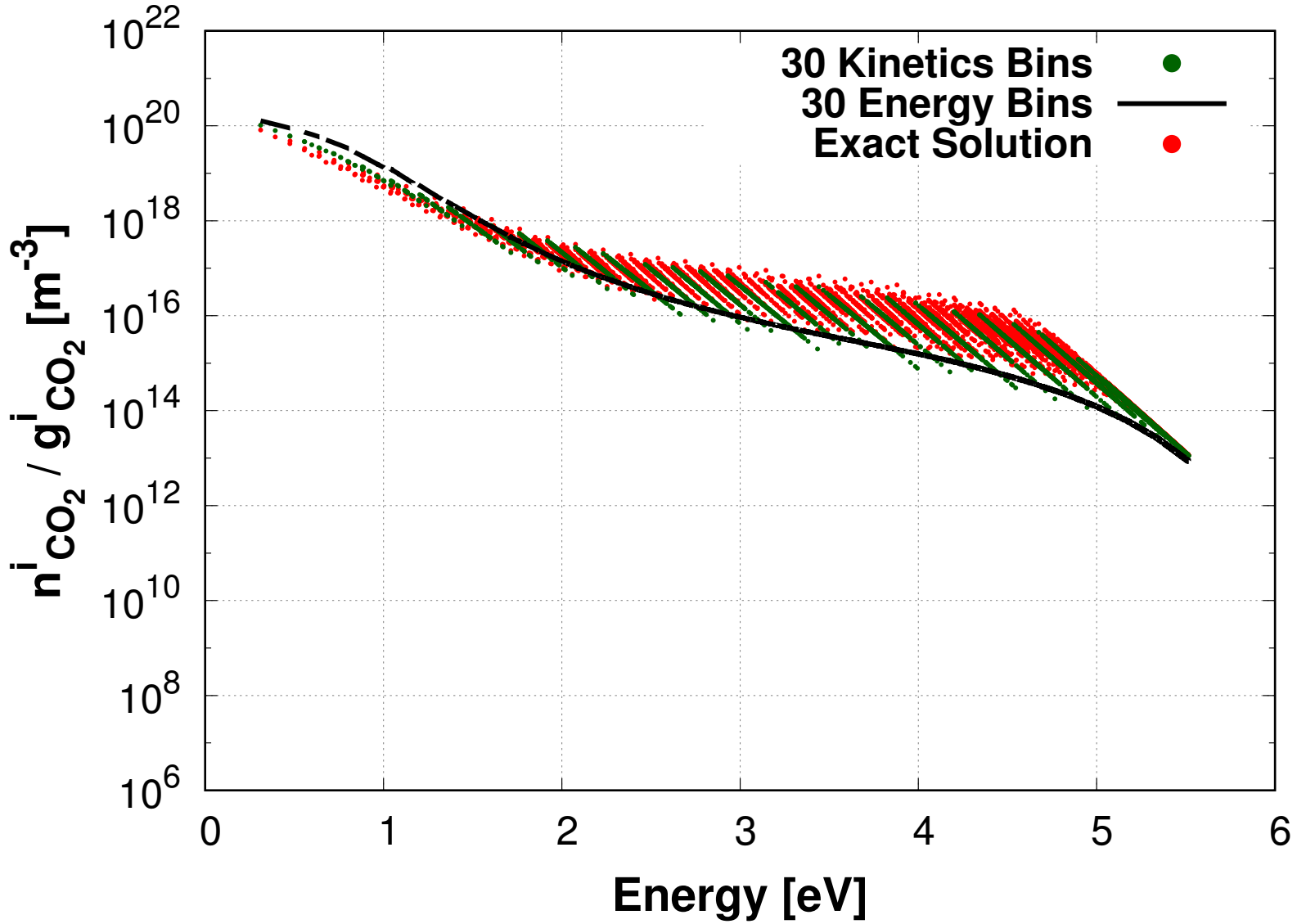
$$\boldsymbol{\Omega} \,.\, \boldsymbol{\nabla} I_g = k^*(\underline{\phi}, \underline{\phi}_0, g)\, a(\underline{\phi}, \underline{\phi}_0, g)\, I_i^{neq}(\underline{\phi}) - k^*(\underline{\phi}, \underline{\phi}_0, k)\, I_g$$

$$\begin{aligned} I_g &= I_k / f(\underline{\phi_0}, \underline{\phi}_0, k) \\ g(\underline{\phi_0}, \underline{\phi}_0, k) &= \int_0^k f(\underline{\phi}_0, \underline{\phi}_0, k)\, dk \\ a(\underline{\phi}, \underline{\phi}_0, k) &= f(\underline{\phi}, \underline{\phi}_0, k) / f(\underline{\phi}_0, \underline{\phi}_0, k) \end{aligned}$$

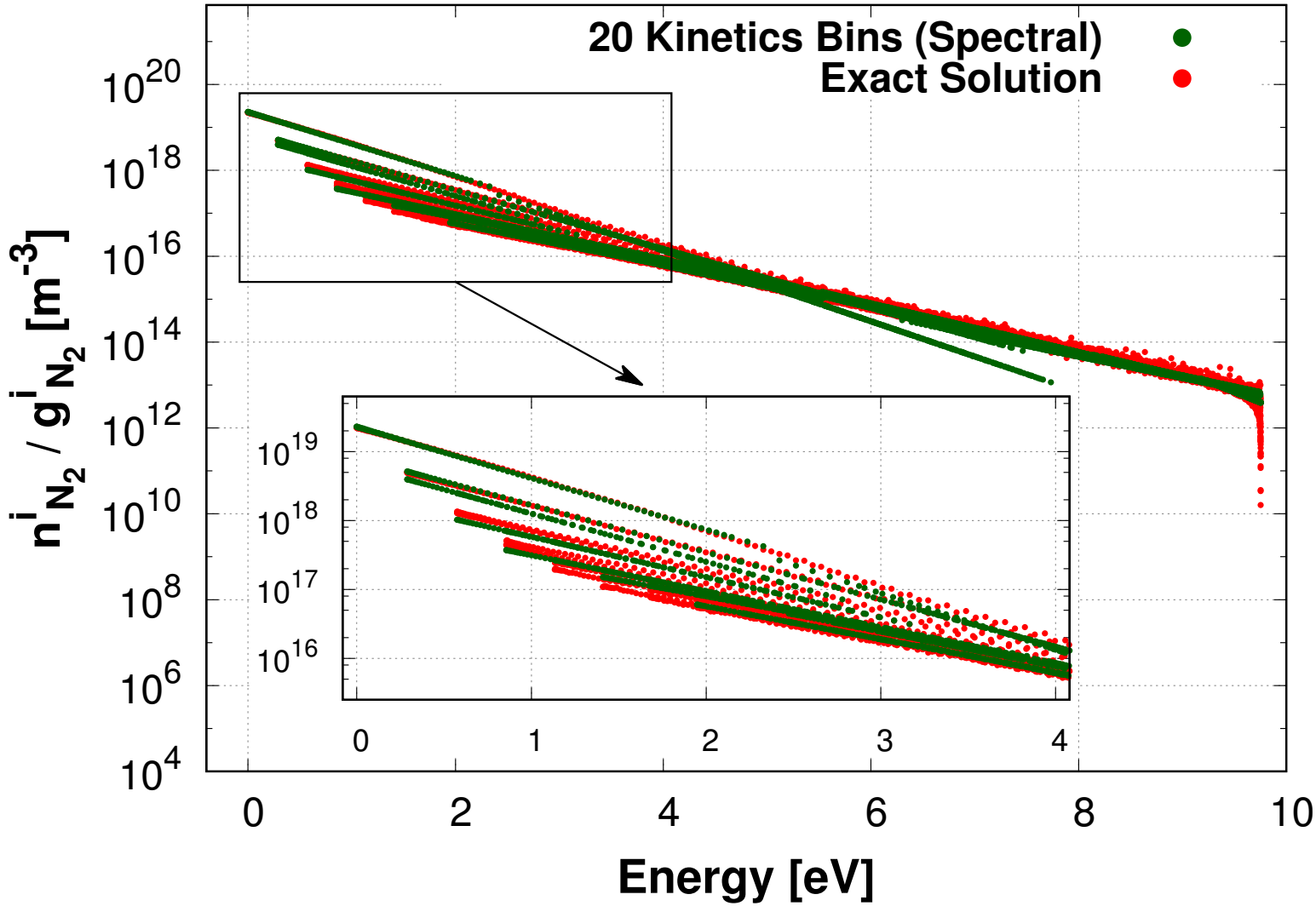
- Integration in g-space performed using numerical quadrature.

$$I_i = \int_0^1 I_g\, dg$$

Spectral Clustering for CO_2



Spectral Clustering for $N_2\left(^1\Sigma_g^+\right) - N\left(^4S_u\right)$



Spectral Clustering for $N_2\left(^1\Sigma_g^+\right) - N\left(^4S_u\right)$