Delivering Breakthrough Solutions

Radiative Transfer Equation Solver Module for Coupled Simulation of Hypersonic Flows

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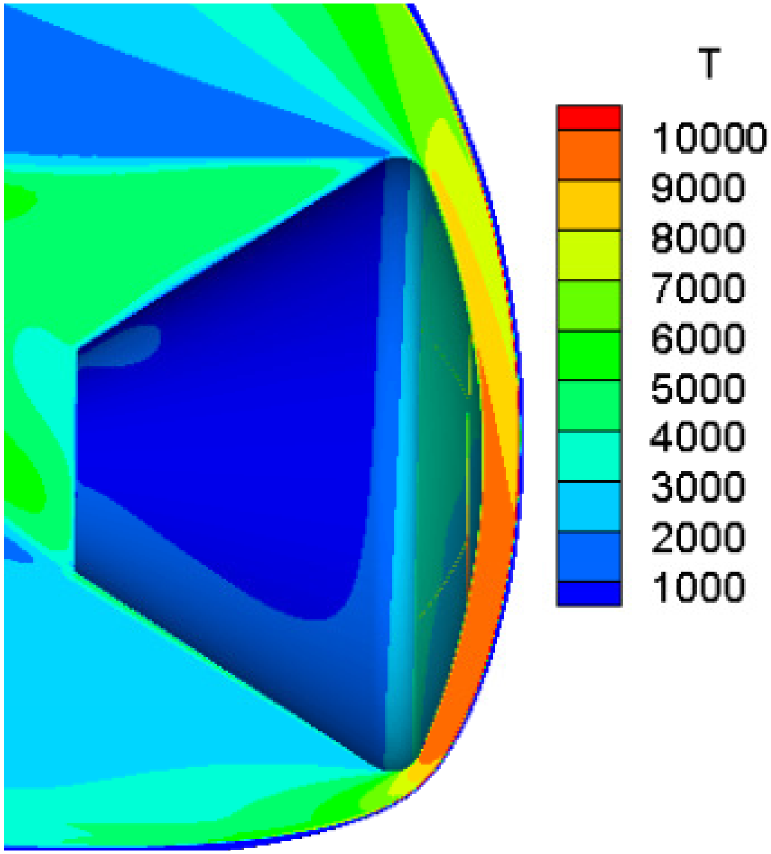
Introduction

1. Work presented is being performed under a joint project between CFDRC, University of Michigan (Prof. Iain Boyd) and University of Kentucky (Prof. Alexandre Martin)
2. Project title: COMPUTATIONAL TOOL FOR COUPLED SIMULATION OF NONEQUILIBRIUM HYPERSONIC FLOWS WITH ABLATION
3. Development of models and model coupling framework
    1. Surface chemistry
    2. Material response
    3. Radiative fluxes
    4. Capturing their interactions and modeling their effects on the ablation phenomena

Accounting for radiative fluxes and solving flow, ablation in a coupled manner should improve model fidelity significantly. That is the main aim of this project

Hypersonic Re-entry

1. Reentry plasma is formed in shock layer in front of the spacecraft entering any atmosphere
2. Many species due to dissociation and ionization: N2, O2 -> O, N, N2+, NO+, etc.
3. Thermochemical nonequilibrium conditions
   - State described not by one but up to four temperatures – T_{tr}, T_{rot}, T_{vib}, T_e
   - Composition = number densities of species and electrons
4. Radiation can contribute 15-80% of the total heat load. Smaller space craft have a lower percentage of heat load from radiation.
5. Need a modular solver framework with accurate radiative properties and RTE solution in multidimensional problems.



Radiation in Hypersonic Plasmas

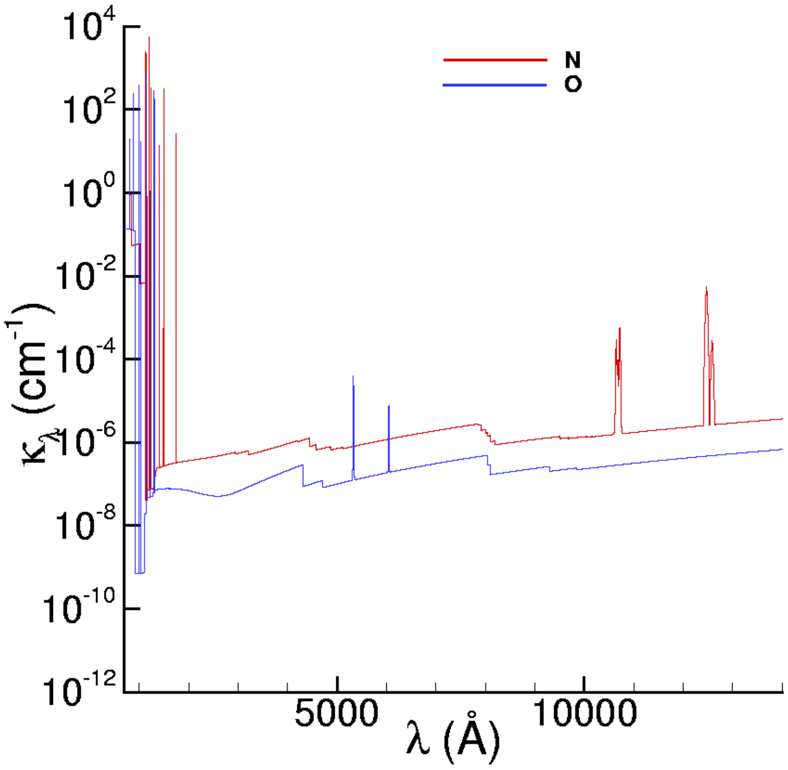
1. Temperatures in the shock layer may exceed 30000K.
2. Nonequilibrium conditions exist. Local emission is not proportional to the absorption coefficient.

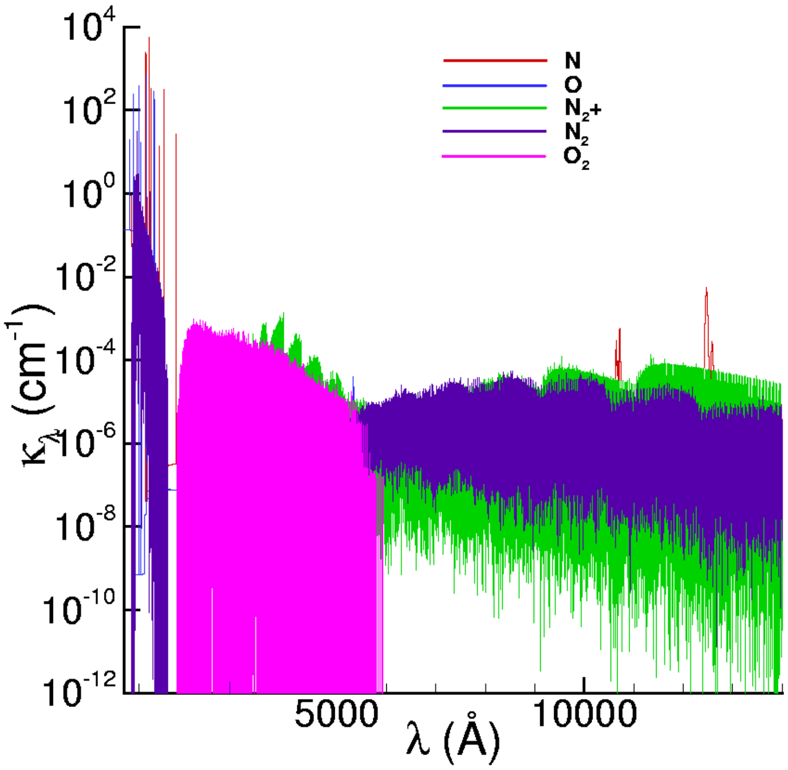
$$\frac{dI_\lambda}{ds} = \varepsilon_\lambda - \kappa_\lambda I_\lambda \quad \left(\varepsilon_\lambda \neq \kappa_\lambda I_{b,\lambda}\right)$$

3. Emission/Absorption due to electronic transitions, and molecular vibrations and rotation : Bound-bound (specific lines), bound-free (continuum) and free-free (continuum) radiation.
4. Line broadening is via Doppler and Lorentz mechanisms. A combined Voigt line shape captures this most accurately.
5. Radiative properties

$$\left(\varepsilon_\lambda, \kappa_\lambda\right) < -(T_{tr}, T_r, T_v, T_e, n_e, n, n^+)$$

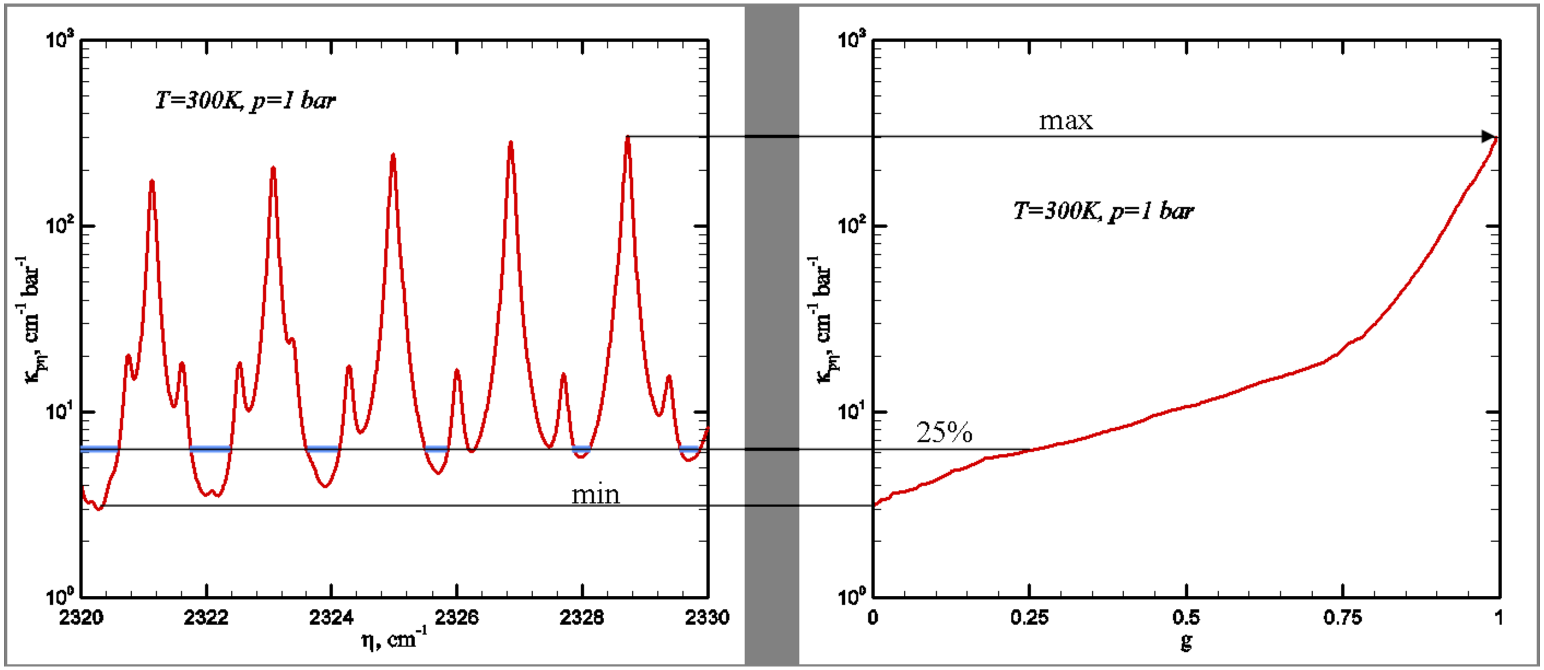
Hypersonic Plasma Spectral Radiative Properties





1. Line-by-line calculations by resolving each line accurately. Spectral width could be as small as 0.005 A° . Approximately 200 key lines for each N and O
2. May need ~35000 RTE evaluations at various spectral lines
3. One-dimensional tangent-slab approximations are tractable using LBL approach, but not multi-dimensional approaches such as P1, which need matrix inversion at each spectral location

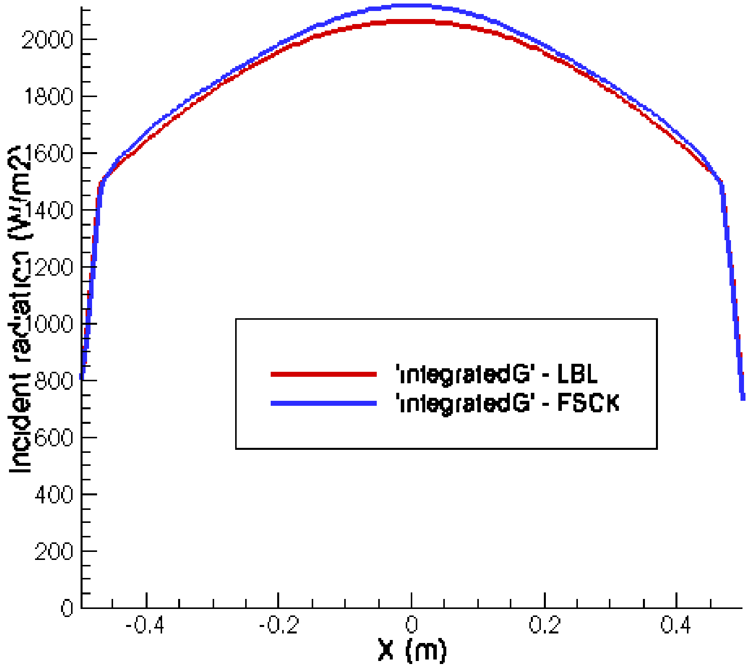
k-distribution based Methods



1. Originally developed by Modest and coworkers for combustion gases – CO2, H2O, CO.
2. Extended to handle inhomogeneous media using multi-group, multi-scale methods [Modest 2003, Pal and Modest 2010]
3. Developed new models for air (earth re-entry) and CO, CN plasma (for Mars re entry).   **Very recent developments Bansal 2011, Bansal and Modest 2009, Bansal and Modest 2010**

Multigroup FSK Method

Description	Units	LBL	k-distribution	
Time to generate properties	(s)	35	19	Per time-step
Solve RTE	(s)	1445	1.1	**1300 speedup**
Accuracy	%	-	**2.7**	



Compact full spectrum and narrow band databases to calculate Full Spectrum *k-distributions on the fly*

Hybrid multi-scale, multi-group FSK: resolves all inhomogeneities

Bansal and Modest developed a high fidelity database for absorption and emission in terms of k-distributions

Spectral integrals are replaced by integrals in the g-space

$$\int_{\lambda} G_\lambda d\lambda = \int_0^1 G_g dg$$

Thus we obtain spectrally accurate results by solving only ~150 scalars in place of ~35000 or more for line-by-line calculations

RTE Solution Methods

1. Photon Monte Carlo
    - Was evaluated in a NASA Phase II with Dr. Rob Rubenstein as COTR
    - Trace few thousand photons per cell to obtain radiation statistics with sufficient accuracy. Need importance sampling or hybrid approaches for better accuracy
2. Spherical Harmonics (P1) Solver
    - Easy to implement, solves a modified Helmholtz equation for direction-integrated radiative intensity
    - Boundary condition of the third-kind
3. Spherical Harmonics with Modified Differential Approximation
    - Separate radiation from medium with radiation from the walls
    - Can improve accuracy significantly particularly for high optical thickness variation. Need complex view-factor calculation and storage framework.
4. Tangent-slab approximation
    - Currently used in DPLR and other similar codes by NASA
    - Calculates 1D solutions along lines with maximum gradient
    - Answers are surprisingly close to those obtained from P1, particularly for small spacecraft
    - Questionable for larger systems, where curvature effects may become important

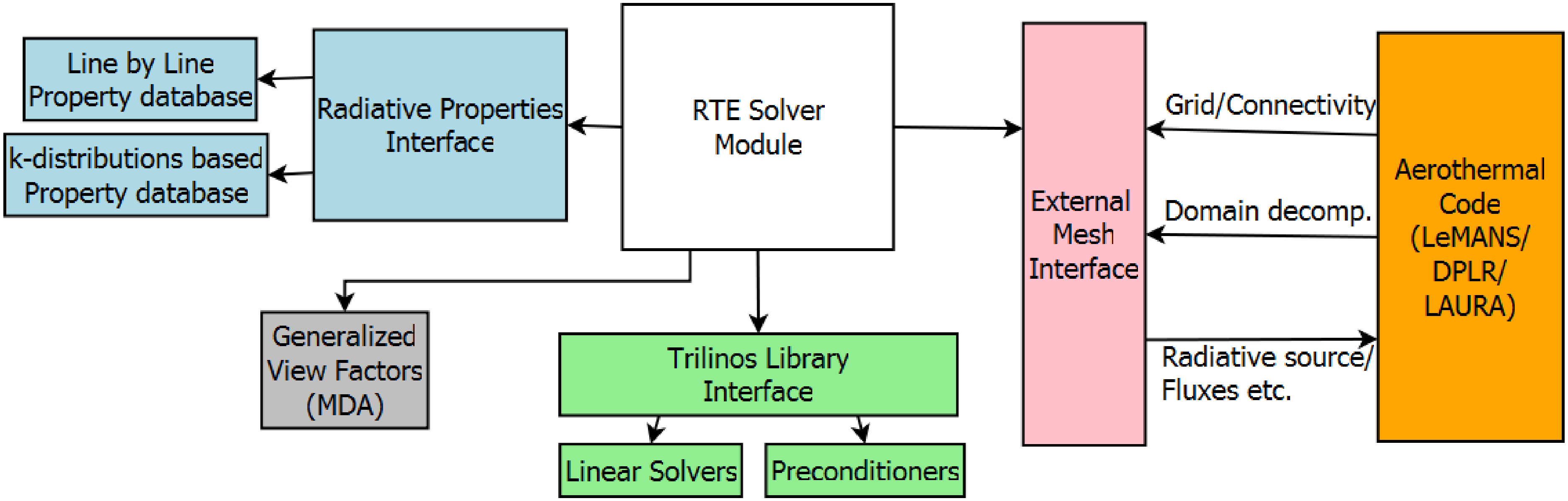
A Modular P1 Solver

1. P1 approximation for direction integrated radiative intensity

$$\nabla\bullet\left(\frac{1}{\kappa}\nabla G\right)-3\kappa G=3\varepsilon \qquad G=\int_{4\pi} I(r,\hat{s})d\Omega$$

2. An MDA solver will be implemented in the next stage of the current project
3. A completely modular and parallelized RTE solver is developed for possible coupling with any CFD aerothermal codes
   - Currently coupled with LeMANS, with planned coupling of MOPAR
   - **Design will allow straightforward coupling of RTE capabilities to any other code for e.g. DPLR**
4. C++ based framework
   - Utilization of Trilinos libraries for completely MPI-based parallelization.
   - Mesh decomposition information is obtained from the CFD Solver to keep flow information local
   - Utilization of Trilinos wrappers for a variety of linear solvers : Currently use Krylov subspace methods with AMG preconditioner.

Modular RTE Solver Architecture



1. Modular structure
2. C++ based classes to implement ExternalMesh, RadiativePropeties
3. The solver has been coupled with LeMANS and can be coupled with other codes of interest such as DPLR, LAURA
4. radSolver has a setRadiativeProperties class to evaluate the absorption coefficient and emission in each cell
5. Domain decomposition same as that used by the flow-solver is SUPPORTED
6. Potentially coarser mesh for radiation, compared to flow solver could be explored

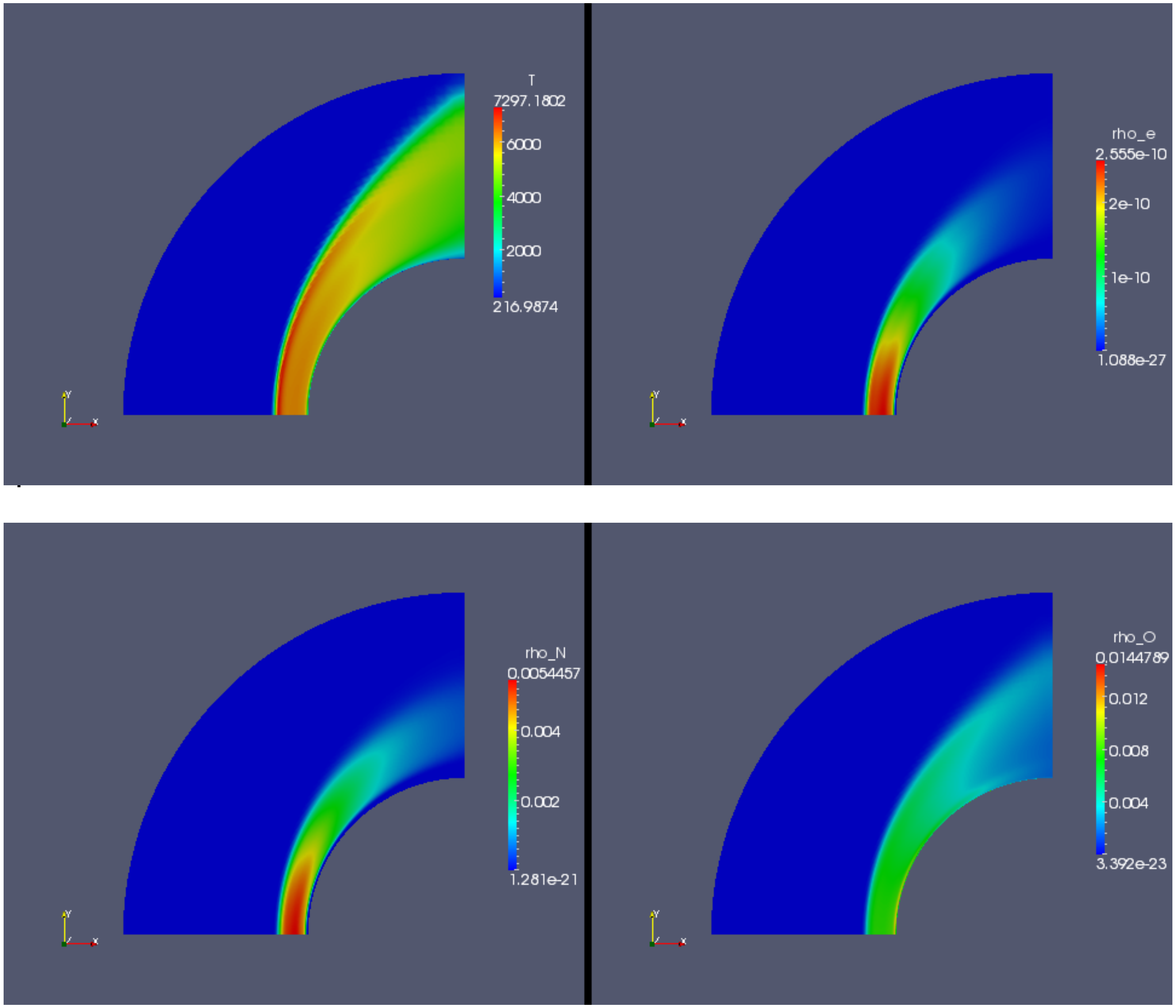
Linear Solver and Preconditioner Study

- 360,000 dof, run on 1 and 8 processors
- Comparison of ILU and AMG preconditioners with GMRES and CGS solvers

#Proc	Solver	PreCond	#iter	CPU (s)
1	GMRES	ILU	102	53.6
1	GMRES	AMG	7	4.7
1	CGS	ILU	69	11.8
1	CGS	AMG	4	4.6
8	GMRES	ILU	142	13.2
8	GMRES	AMG	8	2.2
8	CGS	ILU	93	10.6
8	CGS	AMG	5	2.3

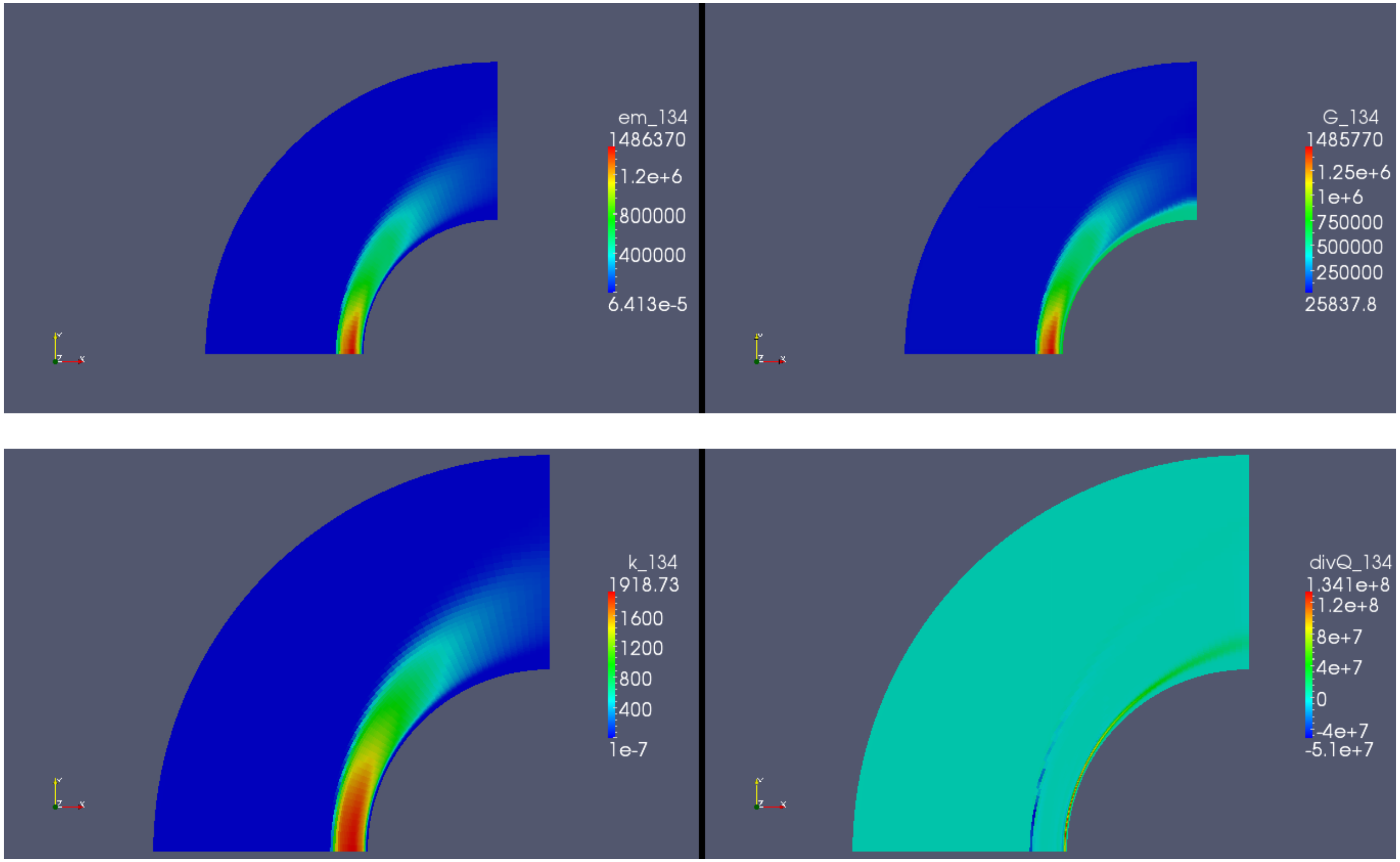
- AMG is more efficient
- AMG requires many fewer solver iterations, especially in parallel
- Switching between solvers and preconditioners done via input file commands

Hypersonic Flow around a Cylinder



1. Cylinder radius 0.25 m
2. Mach 29 flow
3. 1 cell thick mesh with symmetry front and back
4. Temperatures ~7300K
5. Flow solver: LeMANS coupled with our RTE solver.

Hypersonic Flow around a Cylinder



1. Radiative emission and irradiation fields (top), absorption coefficient and divergence of radiative flux (bottom). Values are reasonable
2. Q of interest: spectrally integrated fluxes at the solid wall for ablation. Framework is almost complete

Conclusions and Future Work

Conclusions

1. Hypersonic flow characterized by nonequilibrium radiation. k-distributions will allow modeling of radiation accurately with markedly lower CPU times
2. Radiative fluxes can be 20-80% of the convective fluxes and can have a deep impact on ablation modeling
3. A modular RTE solver framework is developed and can be reused with multiple different codes as required.
4. Demonstration of a flow around cylinder case is done by coupling with LeMANS code.

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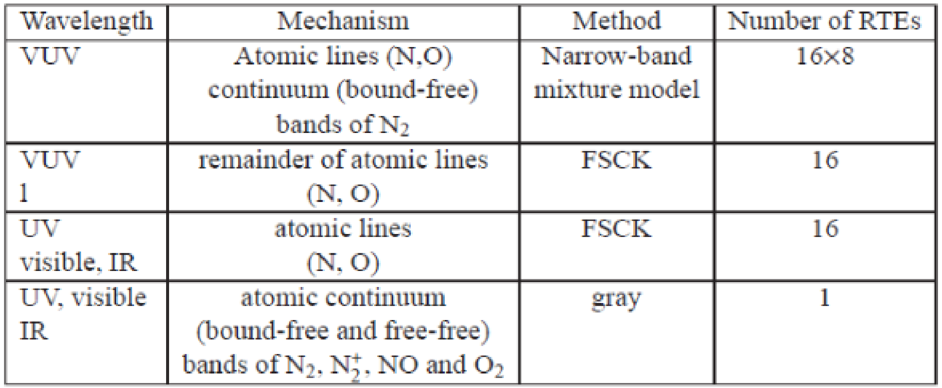
Future Work

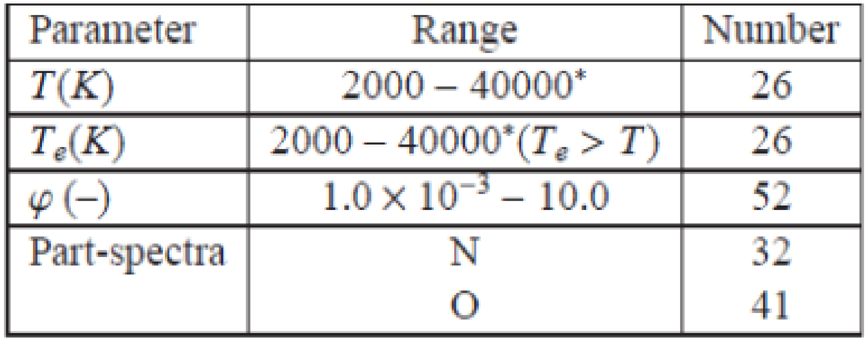
1. Development and implementation of the MDA extension of the P1 method
2. Coupling with material response code to really bring out role of radiation
3. Detailed validation of the methodology in a coupled formulation and separating various interaction effects.
4. Including ablated species/material: Material properties, non gaseous material distribution, including liquid droplets etc.
5. Incorporating detailed spectral effects : escape factors etc.

Multigroup FSK Method

1. Compact full spectrum and narrow band databases to calculate Full Spectrum *k-distributions on the fly*
2. Multi-scale FSK to resolve spatial concentration inhomogeneities
3. Multi-group FSK to resolve spatial temperature inhomogeneities
4. Hybrid multi-scale, multi-group FSK: resolves all inhomogeneities



Wavelength	Mechanism	Method	Number of RTEs
VUV	Atomic lines (N,O) continuum (bound-free) bands of N_2	Narrow-band mixture model	16×8
VUV 1	remainder of atomic lines (N, O)	FSCK	16
UV visible, IR	atomic lines (N, O)	FSCK	16
UV, visible IR	atomic continuum (bound-free and free-free) bands of N_2, N_2^+, NO and O_2	gray	1



Parameter	Range	Number
$T(K)$	$2000 - 40000^*$	26
$T_e(K)$	$2000 - 40000^*(T_e > T)$	26
$\varphi\,(-)$	$1.0 \times 10^{-3} - 10.0$	52
Part-spectra	N O	32 41

Example: Virtual Mesh Interface

```
class ExternalMesh {
  virtual int getNumNodes() = 0;
  virtual int getNumFaces() = 0;
  virtual int getNumCells() = 0;

  virtual void getPartitionMap(int **pMap) = 0;
  virtual void getFaceNodes(int i, int n[4]) = 0;
  virtual void getFaceCells(int i, int &cl, int &cr) = 0;
  virtual void getCellNodes(int i, int n[8]) = 0;
  virtual void getCellFaces(int i, int f[6]) = 0;
};
```

ExternalMesh class defines the interface between the radiation solver and the CFD code. The CFD mesh will inherit this class and provide the pure virtual functions, providing mesh integration between the 2 codes.