

11TH RHTG WORKSHOP · MOLA DI BARI · 23 SEPTEMBER 2026

HelioSPARK

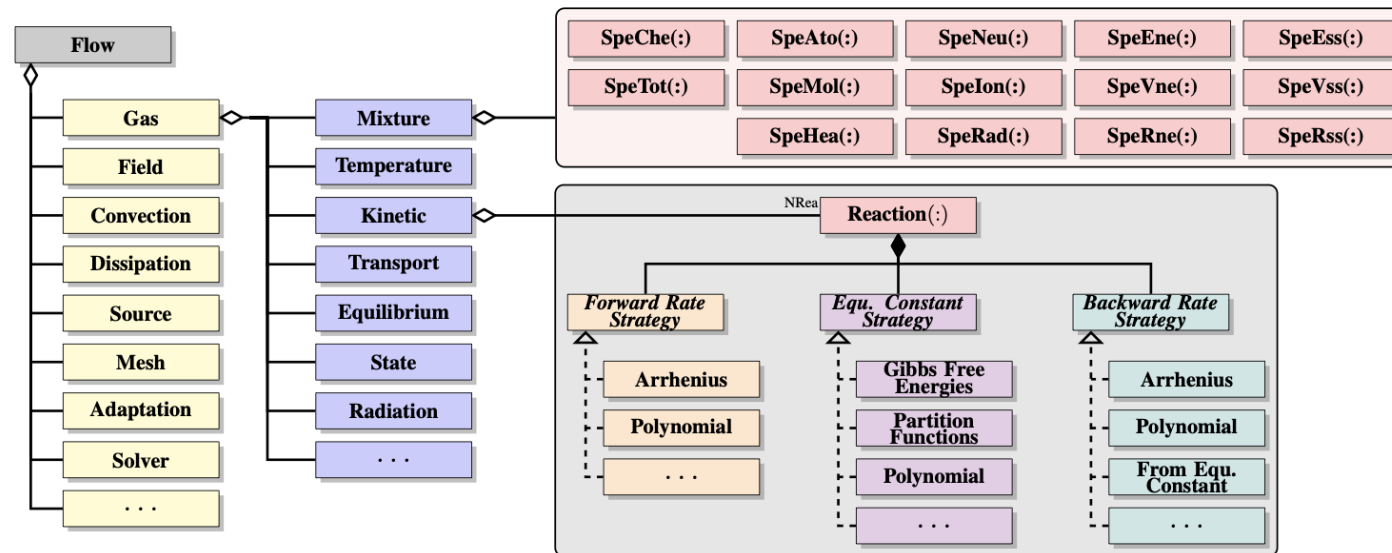
A modular CFD solver for thermochemical
nonequilibrium hypersonic flows

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SPARK – Software Package for Aerothermodynamics, Radiation and Kinetics



SPARK object model: flow, gas mixture and kinetic-rate hierarchy

SPARK CFD

a CFD code for the modelling of entry plasmas. It is OOP (object oriented programming).

SPARK – Radiation

a line-by-line radiative code ranging from the VUV to the IR regions.

Lopez, B., Lino da Silva, M., SPARK: A Software Package for Aerodynamics, Radiation and Kinetics, AIAA 2016-4025.

HelioSPARK

- 1 SPARK current limitations motivated the choice of AMReX. Fortran is less convenient than C++ for building a modern MPI/GPU-native CFD solver
- 2 As starting point, a new solver was developed using AMReX fluid templates, allowing a scalable, modular and AMR-capable framework
- 3 This decision was motivated by computational needs (MPI, HIP, CUDA, etc).



Inspired by god of sun Helios



AMReX as backbone



Toward exascale computing

HelioS solves the multi-species Navier–Stokes system with one conservation equation per internal energy pool

Mass

$$\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}) = 0$$

Species ($s = 1 \dots N_s$)

$$\partial \rho_s / \partial t + \nabla \cdot (\rho_s \mathbf{u}) = -\nabla \cdot \mathbf{J}_s + \dot{\omega}_s$$

Momentum

$$\partial (\rho \mathbf{u}) / \partial t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) = \nabla \cdot \boldsymbol{\tau}$$

Total energy

$$\partial (\rho E) / \partial t + \nabla \cdot [(\rho E + p) \mathbf{u}] = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q} - \nabla \cdot \sum_s h_s \mathbf{J}_s$$

Energy pools ($m = 1 \dots N_p$)

$$\partial (\rho e_m) / \partial t + \nabla \cdot (\rho e_m \mathbf{u}) = -\nabla \cdot \mathbf{q}_m - \nabla \cdot \sum_s e_{m/s} \mathbf{J}_s + \Omega_m$$

Notation

ρ, ρ_s mixture and species density
 $\mathbf{u}, p, \boldsymbol{\tau}$ velocity, pressure, viscous stress
 $E = e + \frac{1}{2}|\mathbf{u}|^2$ total specific energy
 e_m energy of pool m (rotational, vibrational, electronic...)
 $\mathbf{J}_s$ species diffusive mass flux
 $\mathbf{q}, \mathbf{q}_m$ total and pool heat flux
 $h_s, e_{m/s}$ species enthalpy and pool energy
 $\dot{\omega}_s$ chemical production rate
 Ω_m pool exchange: VT, VV, e-heavy, chemistry, radiation

Pools are data, not code: 1T (no pool equation), 2T (one vibrational–electronic pool) and 3T are the same solver with a different EnergyPoolModel, while T4 includes all energies pools. Closure: NASA-9 thermodynamics, Gupta–Yos / Wright transport, finite-rate chemistry.

Time advance is second-order Strang splitting over three operators, arranged S-D-H-D-S



S Sources

Finite-rate kinetics and energy-pool relaxation. Stiff ODE per cell, integrated by SUNDIALS CVODE.

D Diffusion

Viscous, thermal, modal and species diffusion. Implicit backward Euler, so it adds no timestep constraint, but can still be under constraint of nonlinearity of problem.

H Hydrodynamics

Explicit finite-volume Godunov. The only CFL-limited operator.

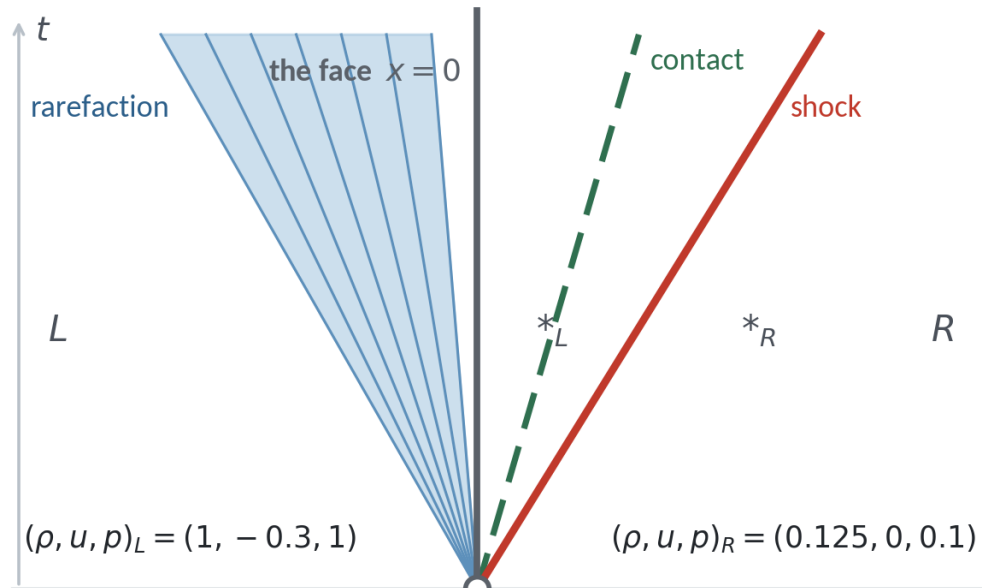
Timestep policy

dt from the hydro CFL condition, ramped from an initial dt and allowed to grow at most $1.2 \times$ per step. A rejected step halves dt and retries. Each operator runs to completion on the state the previous one produced; the symmetric arrangement gives second order.

The Riemann problem at every face

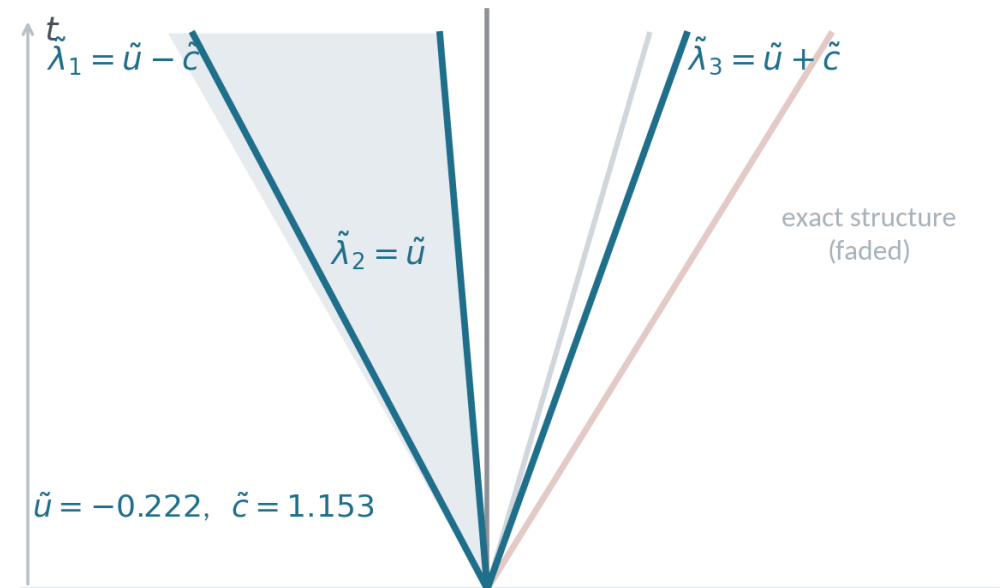
A finite-volume step needs a flux where two different states meet.

(a) The exact solution



Exact: $p^* = 0.2520$, $u^* = 0.7573$ — the face lies in the left star region.
Doing this nonlinearly at every face and every step is far too expensive.

(b) Roe: three straight waves



One algebraic pass, no iteration — cheap and sharp. But a sonic rarefaction admits an expansion shock: hence the entropy fix.

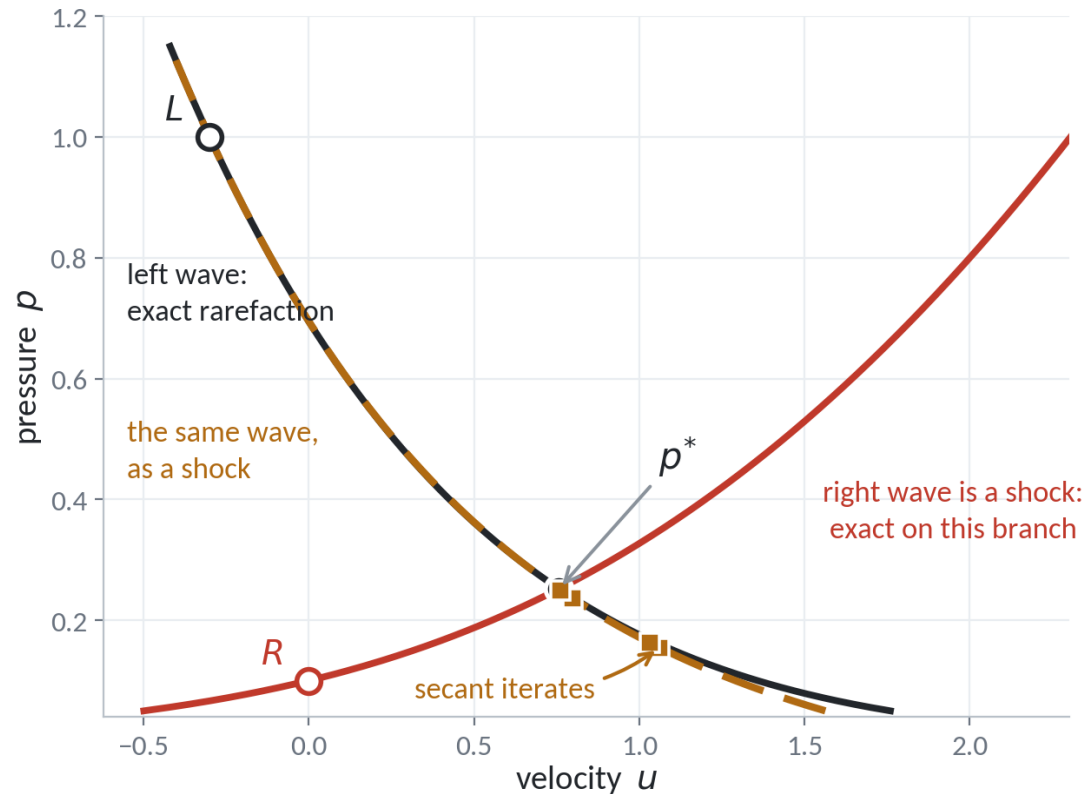
$$F = \frac{1}{2}(F_L + F_R) - \frac{1}{2} \sum_k |\tilde{\lambda}_k| \alpha_k \tilde{r}_k, \quad \alpha_k = \tilde{l}_k \cdot (U_R - U_L), \quad F_R - F_L = \tilde{A} (U_R - U_L)$$

The Roe average is built so the last identity holds exactly — that is what makes the linearized solver conservative.

Colella–Glaz: two shocks, solved for p^*

The nonlinearity is kept: both waves are modelled by the shock relations, and p^* is found by iteration.

The two wave curves in the p – u plane



Only the left branch is approximated: the right wave really is a shock, so the two-shock relation is exact there.

How it works

Each wave is replaced by its shock relation, so the star state is where the two curves meet:

$$\frac{p^* - p_L}{W_L} + \frac{p^* - p_R}{W_R} = u_L - u_R$$

$$W_K = \sqrt{\rho_K \left[\frac{\gamma + 1}{2} p^* + \frac{\gamma - 1}{2} p_K \right]}$$

W depends on p^* , so p^* comes from a secant iteration — 2 to 4 passes. For a real gas γ becomes a local γ_{eff} from the EOS: that is the 1985 paper.

For this Riemann problem

$$p^* \text{ exact} = 0.2520, \quad u^* = 0.7573$$

$$p^* \text{ two-shock} = 0.2517, \quad u^* = 0.7561$$

$$\Rightarrow 0.13\% \text{ error on } p^*$$

The state at $x/t = 0$ is then sampled from the wave pattern and the flux evaluated once: $F = F(U^*)$.

Same job, different bargain

Both solvers take the same two states and hand back a flux. They differ in what they approximate, and in how they fail.

	Roe (1981)	Colella–Glaz (1985)
<i>approximates</i>	the Jacobian, linearized about a Roe average	the two nonlinear waves, both treated as shocks
<i>solved by</i>	one algebraic pass, no iteration	secant iteration on p^* (2–4 passes)
<i>returns</i>	the interface flux directly	the state at $x/t = 0$, then $F = F(U^*)$
<i>weak spot</i>	sonic rarefaction; negative p or p	rarefactions as shocks; vacuum needs a fallback
<i>real gas</i>	the Roe average must be rebuilt per EOS	general convex EOS via a local γ_{eff}

Roe is the sharpest and the cheapest and needs an entropy fix plus a positivity fallback to survive strong expansions.

Colella–Glaz is sturdier where the shocks are strong and the gas is not ideal.

HelioS also has a non-iterative variant, CG–Ferguson, and falls back to full Colella–Glaz when it fails.

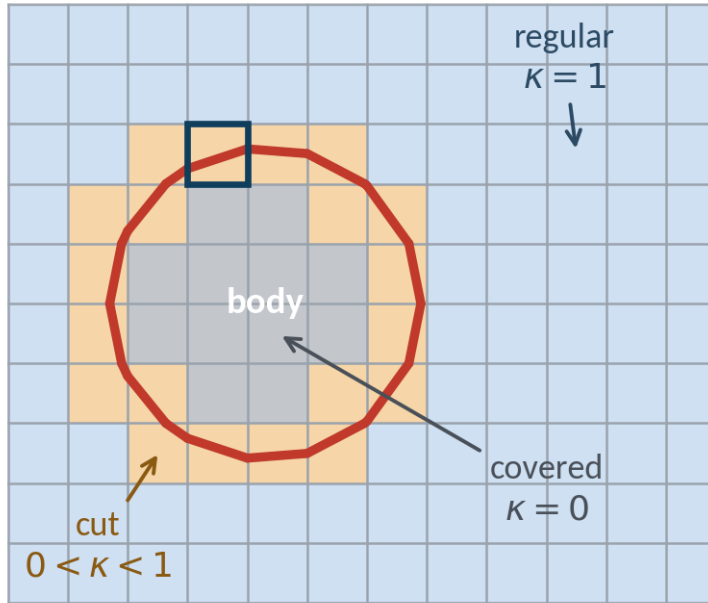
Both carry the contact, so both keep shear and material interfaces sharp and both can carbuncle on a grid-aligned bow shock.

Roe, JCP 43 (1981) 357–372 • Colella & Glaz, JCP 59 (1985) 264–289 • Colella & Woodward (PPM), JCP 54 (1984) 174–201

Embedded boundary (EB) methods

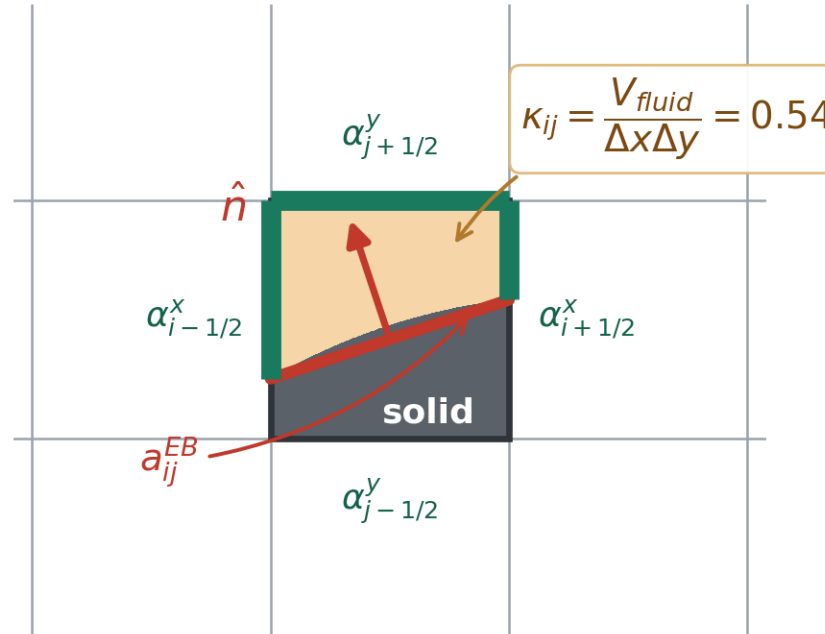
The body is embedded in a fixed Cartesian grid; the cells it cuts stay in the solution.

Regular, cut, covered



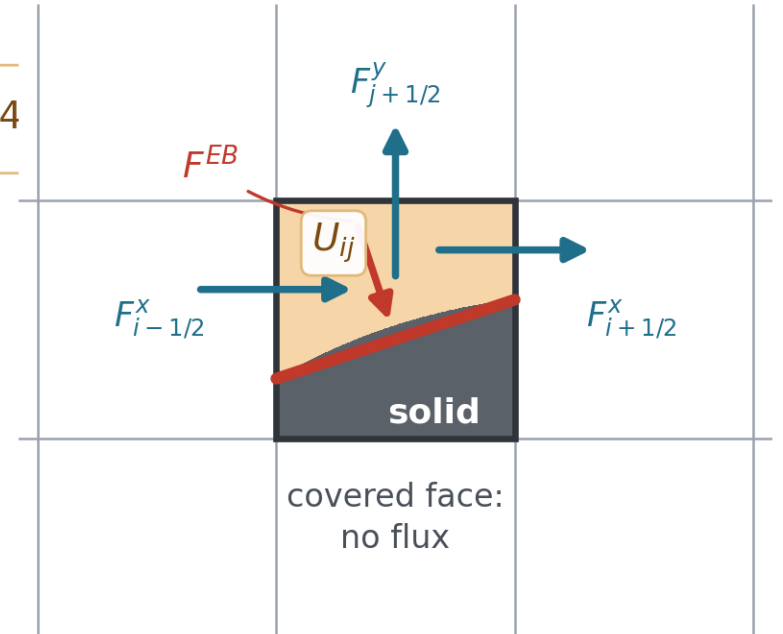
One grid, built without regard for the body.
Red: one planar EB facet per cut cell.

A cut cell in numbers



κ : fluid volume. α : open part of a face (green).
The facet carries its own area and normal.

Conservation, fluid part only



Flux crosses only the open part of a face;
the wall adds one more, carrying the BC.

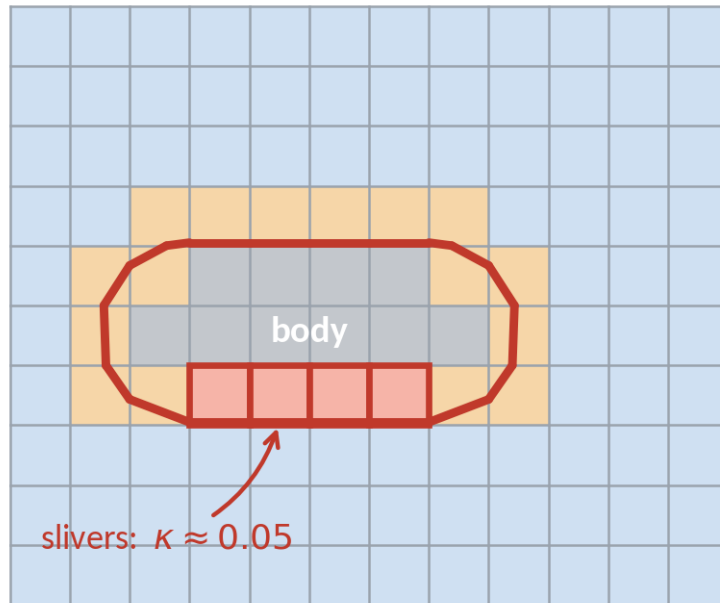
$$\kappa_{ij} \frac{dU_{ij}}{dt} = -\frac{1}{\Delta x} (\alpha_{i+1/2}^x F_{i+1/2}^x - \alpha_{i-1/2}^x F_{i-1/2}^x) - \frac{1}{\Delta y} (\alpha_{j+1/2}^y F_{j+1/2}^y - \alpha_{j-1/2}^y F_{j-1/2}^y) - \frac{a_{ij}^{EB}}{\Delta x \Delta y} F_{ij}^{EB}$$

A regular cell has $\kappa = \alpha = 1$ and no EB face, which recovers the standard scheme: the geometry enters only through these numbers.

The small-cell problem

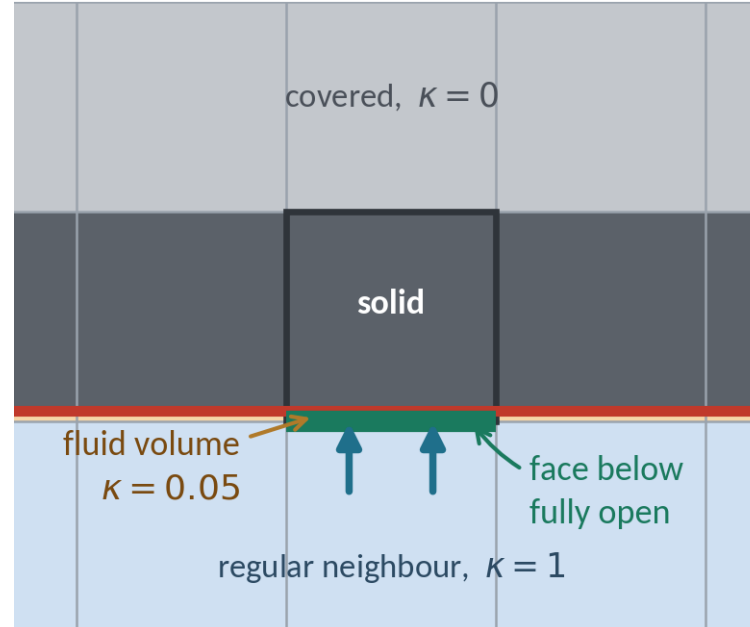
An explicit update divides the incoming fluxes by the cell's fluid volume.

The wall can graze a face



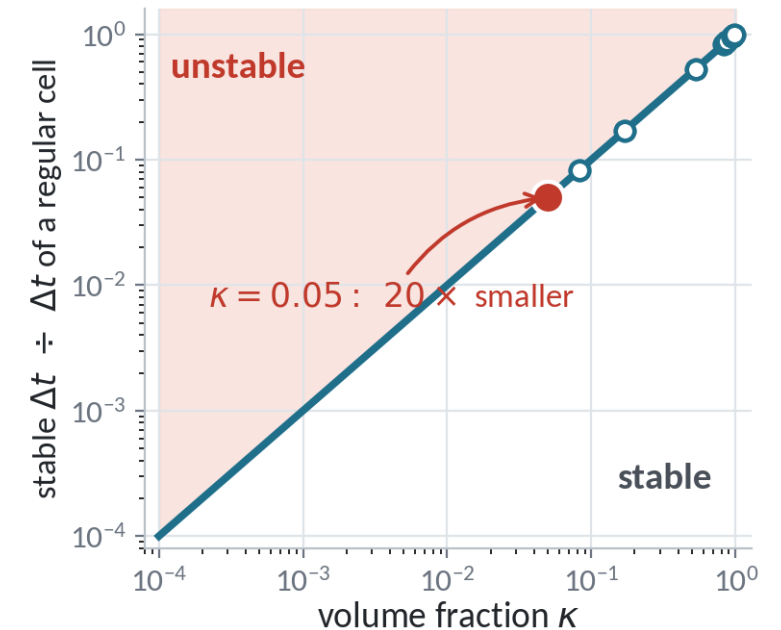
κ is whatever the geometry gives; refining the grid only relocates the slivers.

No volume, full-size faces



An $O(1)$ flux enters a cell holding 5% of one. In real geometries $\kappa = 10^{-3}$ is routine.

The time step collapses



Circles: every cut cell at left. One sliver sets the step for the whole domain.

$$\Delta t \leq \frac{K_{ij}}{\alpha_{max}} \frac{\Delta x}{|u| + c} \approx K_{ij} \Delta t_{regular}$$

$$U^{n+1} = U^n - \frac{\Delta t}{\kappa \Delta x} (\dots)$$

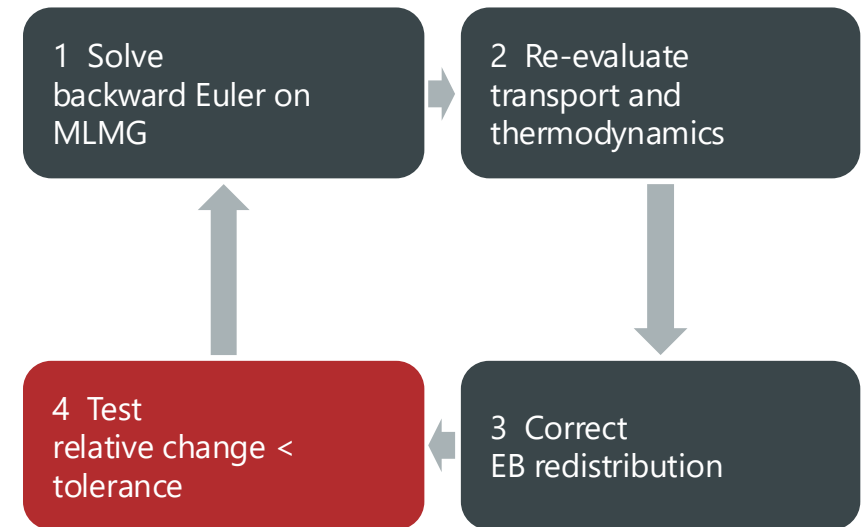
The cures give the sliver an $O(1)$ volume: flux redistribution • state redistribution • cell merging • implicit cells

Diffusion is implicit: backward Euler on AMReX multigrid, wrapped in a Picard loop

Diffused quantity	Operator	Form
Temperatures (per pool)	MLEBABecLap	scalar, $A \cdot T - dt \nabla \cdot (B \nabla T)$
Species mass fractions	MLEBABecLap	scalar, one solve per species
Momentum (viscous)	MLEBTensorOp	tensor, full stress
Without embedded boundaries	MLABecLaplacian / MLTensorOp	same, no cut cells

Explicit path also available (forward Euler or adaptive SSPRK2 with substepping) where the implicit machinery is not wanted.

Picard fixed-point iteration



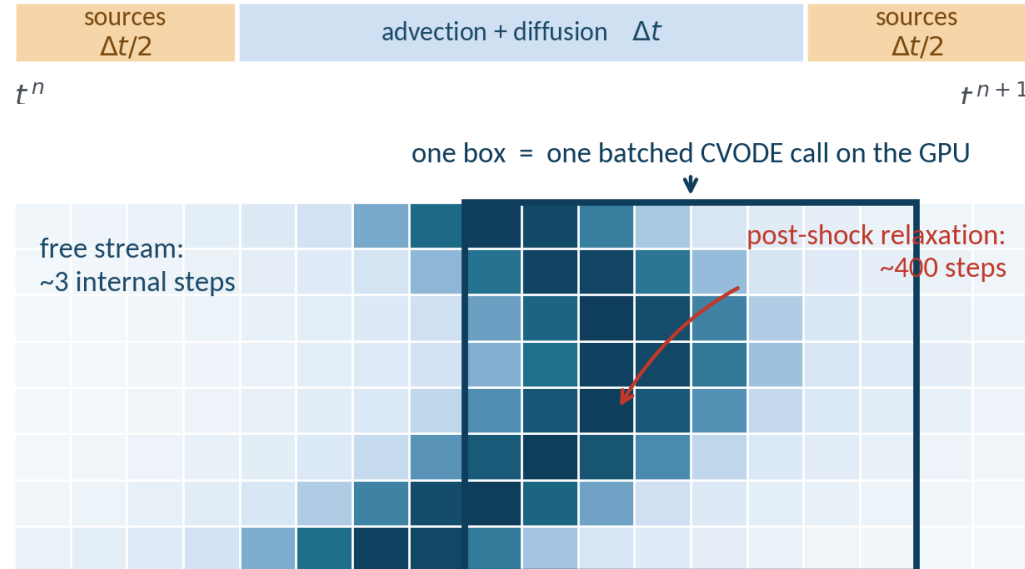
Convergence test is the maximum of three quantities

State change, species-consistency residual, and change in the redistribution correction. In practice the third is frequently the one that limits convergence.

Stiff sources: chemistry and energy transfer, cell by cell

Reactions and modal energy relaxation carry no spatial derivatives, so the split leaves one stiff ODE system per cell for CVODE.

Split the step, then solve each cell on its own



Colour: CVODE internal steps per cell in one source half-step. Each cell picks its own substeps; only the batch boundary is shared.

$$\mathbf{y} = [\rho Y_1 \dots \rho Y_{N_s}, \rho e_v, \rho e_e]$$

$N_s + 2$ unknowns per cell: 11-species air gives a dense 13×13 Jacobian block per cell.

The system in each cell

$$\frac{d(\rho Y_k)}{dt} = \dot{\omega}_k(\rho, \mathbf{Y}, T, T_v, T_e)$$

$$\frac{d(\rho e_v)}{dt} = \Omega_{VT} + \Omega_{VV} + \Omega_{eV} + \Omega_{CV}$$

$$\frac{d(\rho e_e)}{dt} = \Omega_{eT} + \Omega_{eV} + \Omega_{ion}$$

Total energy is fixed: transfer terms move energy between modes, never create it.

What makes it stiff — and coupled

$10^{-9} - 10^{-2}$ s

relaxation-time span, shifting by orders of magnitude across the shock layer

V–T, V–V, e–V, e–T, ionization and chemistry–vibration coupling on $T_a = \sqrt{(T \cdot T_v)}$: one dense block

How AMReX runs it

CPU

One CVODE problem per cell

GPU

One N_Vector per box; the batch moves at its stiffest cell's pace

AMR lifts the implicit operators out of time subcycling: 6 diffusion solves per step instead of 14

Standard Berger–Colella path (recursive subcycling)

Each level advances a complete Strang step, then calls the next finer level ref_ratio times at $\text{dt}/\text{ref_ratio}$. Coarse–fine boundaries filled by `FillPatchTwoLevels` with time interpolation; fluxes captured in `FluxRegister` / `EBFluxRegister`, refluxed on unwind; fine solution averaged down.

Level 0	dt			
Level 1	dt/2		dt/2	
Level 2	dt/4	dt/4	dt/4	dt/4

Three-level 2:2 hierarchy: $1 + 2 + 4 = 7$ level-steps per coarse step, so 14 half-step diffusion solves; common timestep needs $2 \times 3 = 6$.

14 diffusion solves per coarse step

Common-timestep path (HelioS)

Hyperbolic operator stays subcycled; sources and diffusion take one dt on all levels at once. An implicit operator carries no Courant constraint, so subcycling it buys nothing and costs the refinement product.



Two variants: axisymmetric runs one composite multigrid solve spanning all levels; Cartesian solves level by level, coarse to fine, with ordinary reflux and average-down (opt-in).

6 diffusion solves per coarse step, 2.3× fewer and 1.9x faster

Checking the code

Three test tiers, separate from the production application

- 1** **Verification/
Diagnostics**
Diffusion conservation, EB thermal ramps, MLMG convergence
- 2** **RegTests/MMS
Per-operator invariants**
One operator at a time, checked against its MMS
- 3** **RegTests/Options/
Coupled behaviour**
Strang cycles and AMR level coupling

Runtime self-checking

- **Admissibility predicates**
on every accepted state
- **Conservation audits**
against flux-register bookkeeping
- **Contract assertions**
on redistribution metadata
- **Per-cell census diagnostics**
on failure

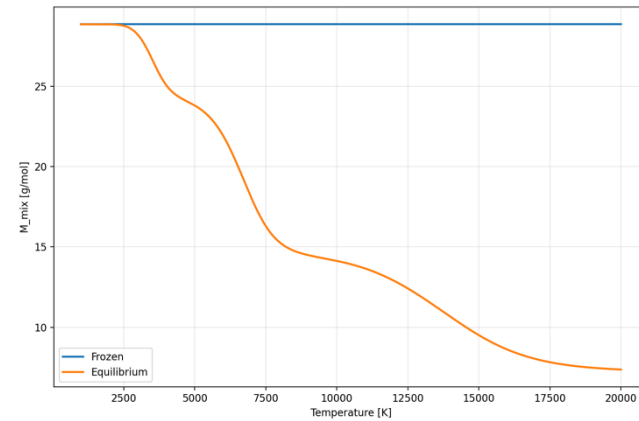
Accelerator readiness **196** device kernels in Diffusion,
Hydro and Sources

37 device kernels in the AMReX layer

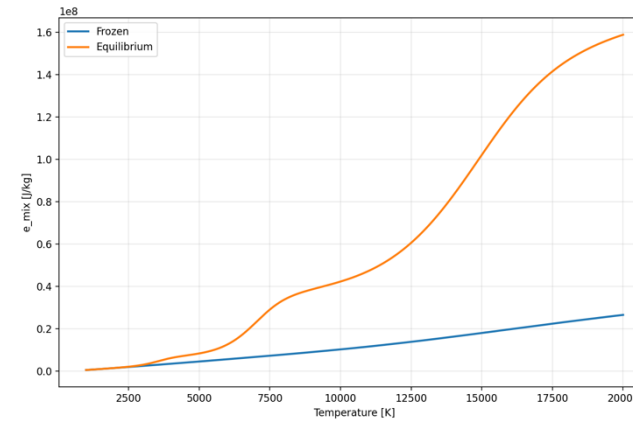
Thermodynamics and transport are still
mostly host-side

Equilibrium air thermodynamics reproduce dissociation and ionisation, with $c_p - dh/dT$ below 0.06 J/kg/K

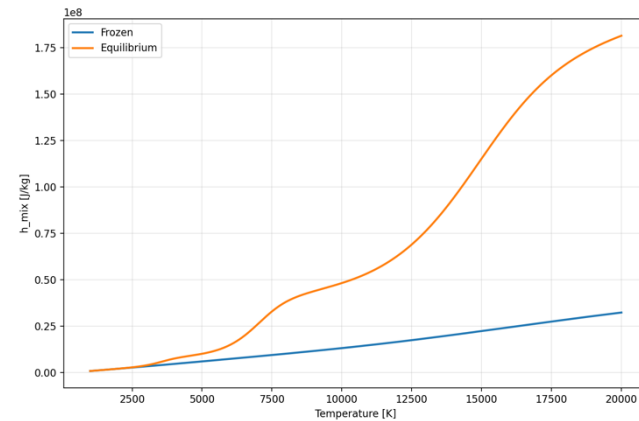
Mixture molar mass, frozen vs equilibrium



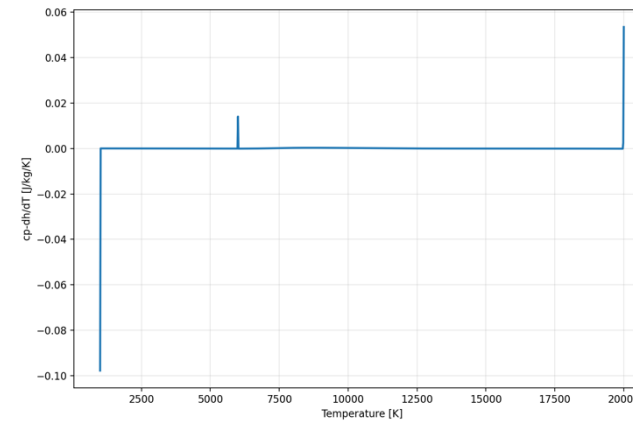
Internal energy, frozen vs equilibrium



Enthalpy, frozen vs equilibrium

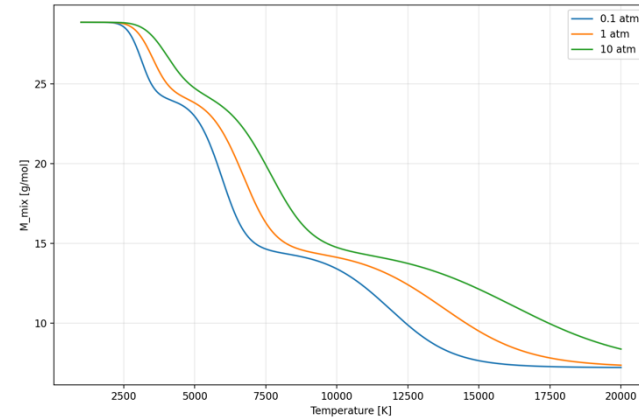


Residual $c_p - dh/dT$

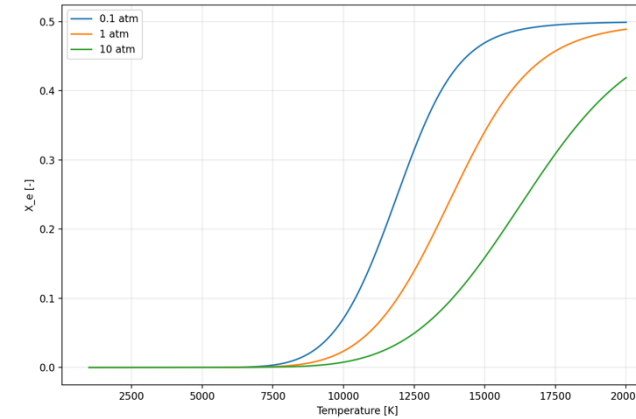


Equilibrium air composition from 1000 to 20000 K

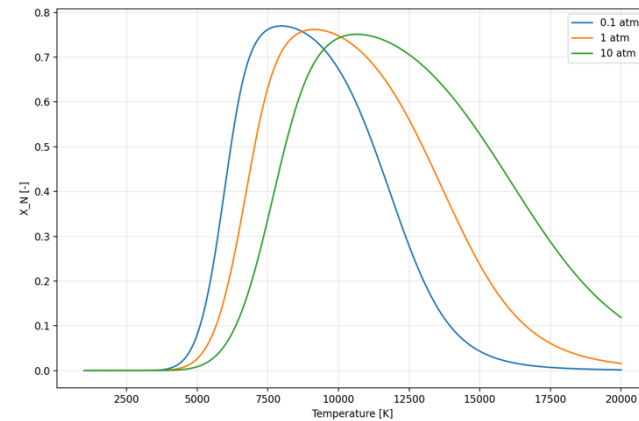
Mixture molar mass, g/mol



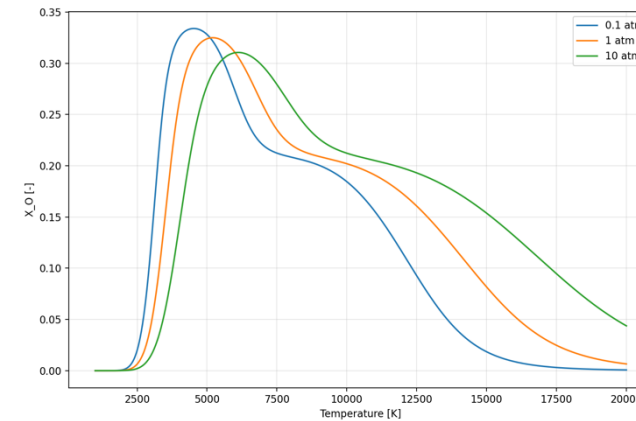
Electron mole fraction X_e



Atomic nitrogen mole fraction X_N



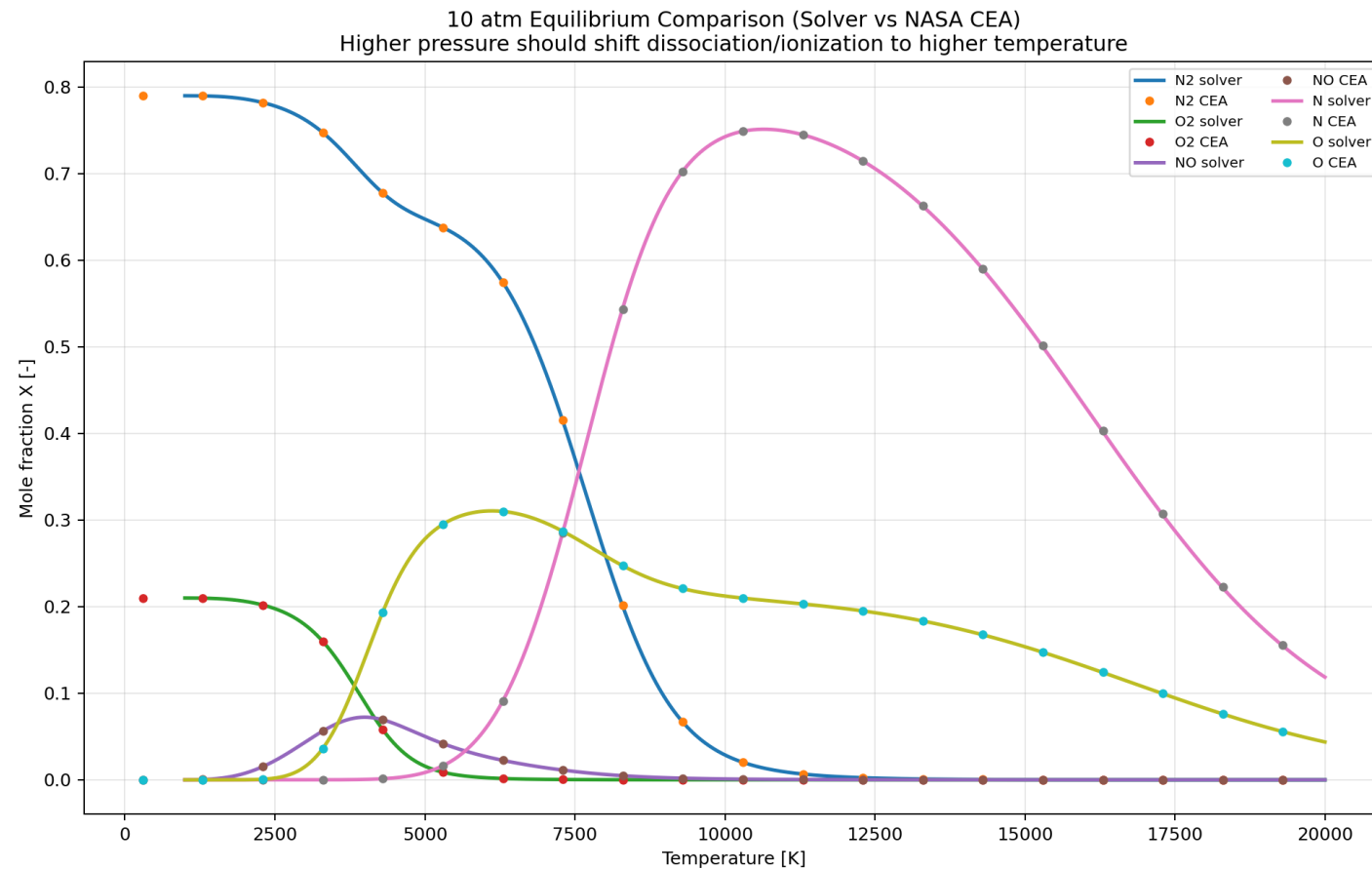
Atomic oxygen mole fraction X_O



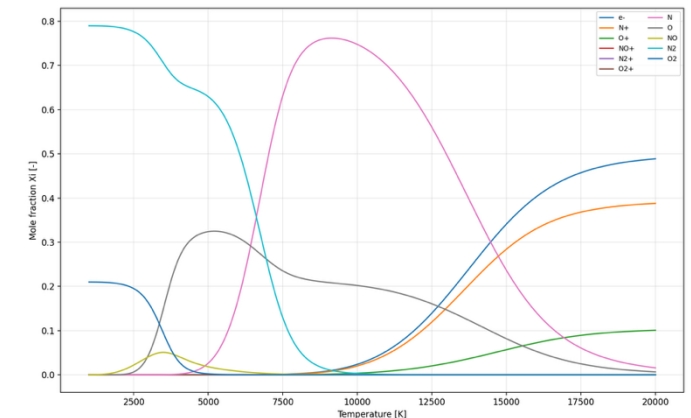
Equilibrium composition at 0.1, 1 and 10 atm from the HelioS thermodynamic database (NASA-9 fits, SPARK species tables).

Equilibrium 11-species air composition matches NASA CEA at 10 atm over the full 1000–20000 K range

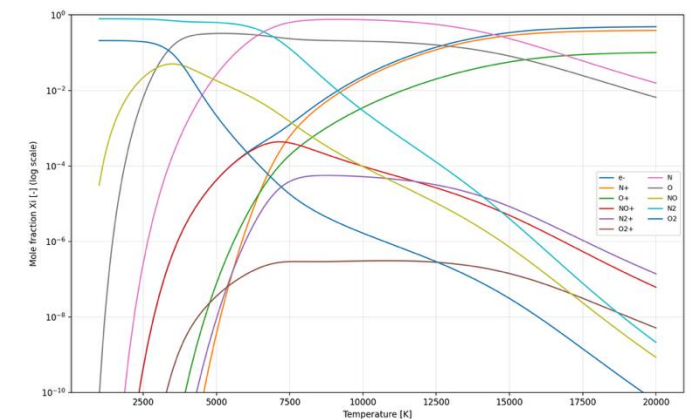
Dominant species at 10 atm, HelioS (lines) vs NASA CEA (points)



11-species composition at 1 atm, linear



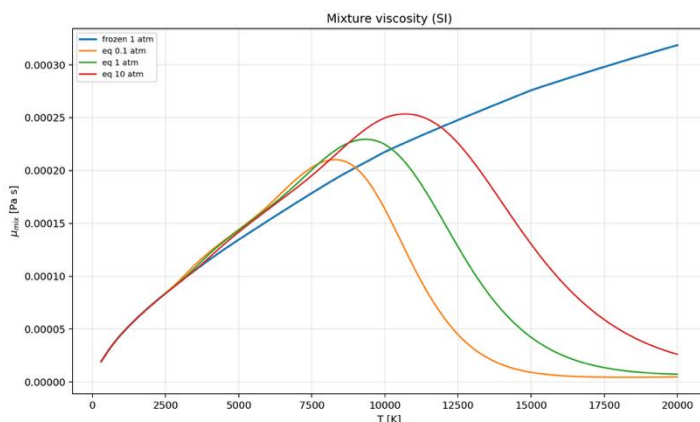
Same data, log scale (trace ions)



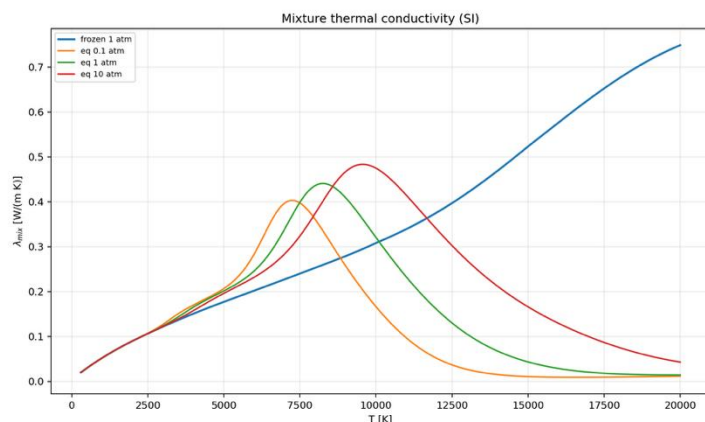
Species: e^- , N, O, NO, N_2 , O_2 , N^+ , O^+ , NO+, N_2^+ , O_2^+ . Reference: NASA CEA (Gordon & McBride) at 10 atm. HelioS equilibrium from the SPARK species tables and NASA-9 fits.

Equilibrium transport properties peak where air dissociates and ionises, then fall an order of magnitude below the frozen values

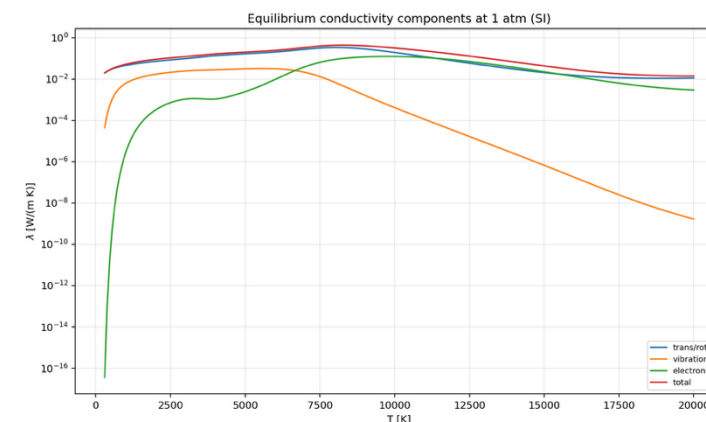
Mixture viscosity μ , Pa·s, frozen vs eq.



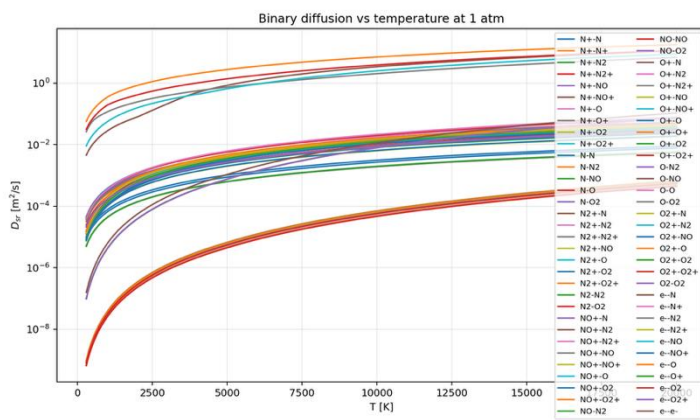
Mixture conductivity λ , W/(m·K), frozen vs eq.



Conductivity components, 1 atm (log)



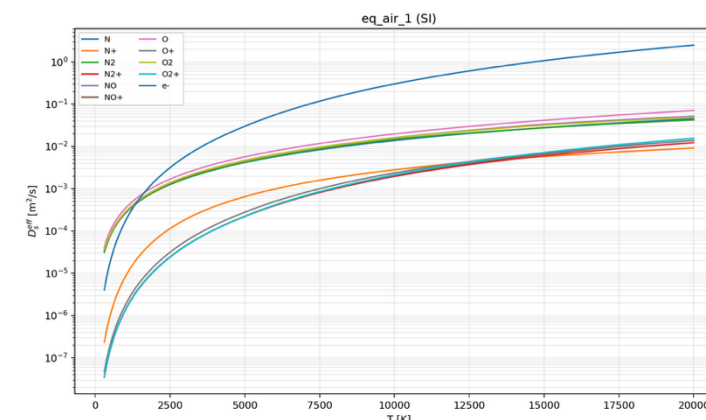
Binary diffusion D_{sr} , all 66 pairs, 1 atm (log)



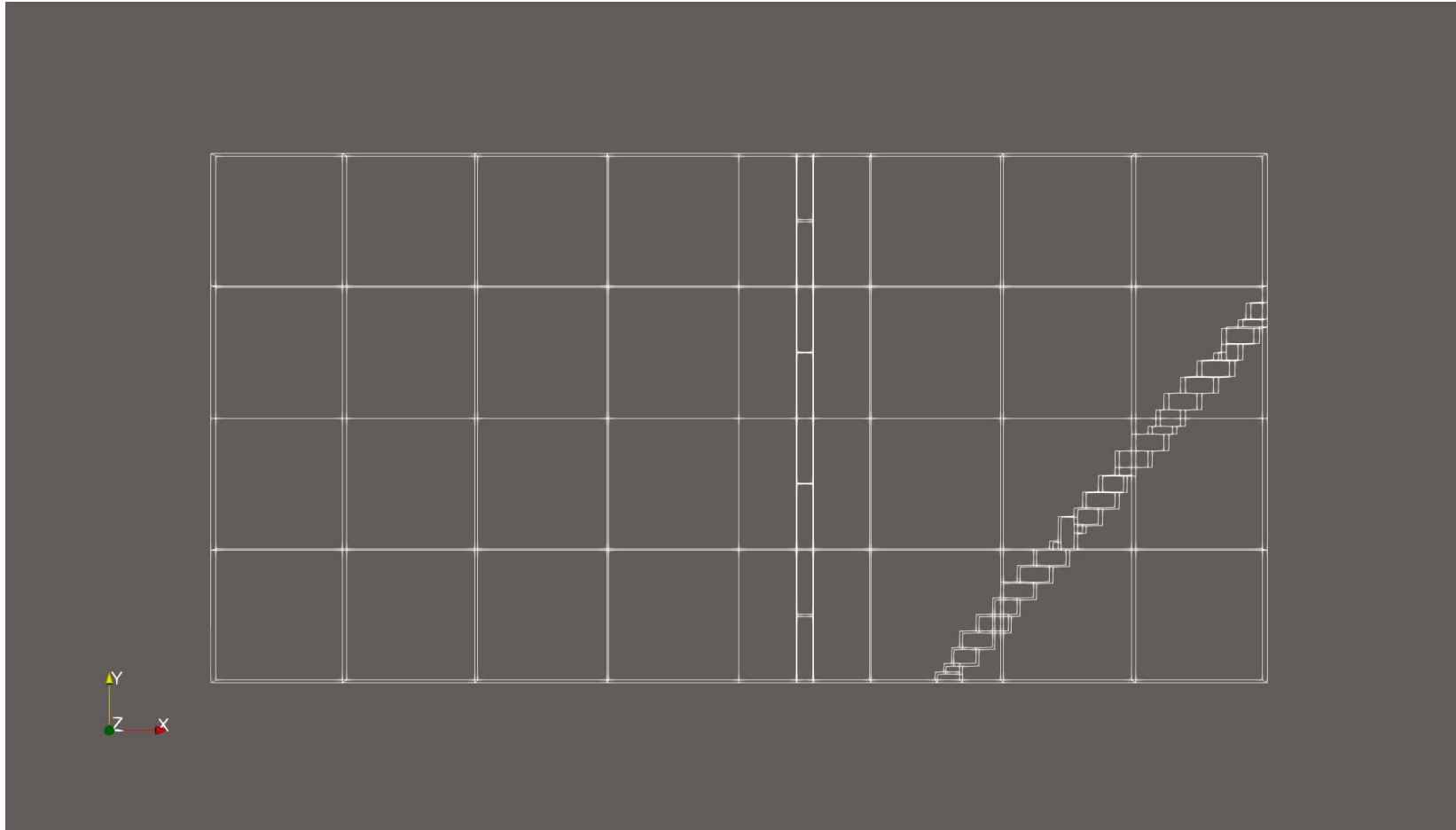
What the curves show

- Frozen μ and λ grow monotonically with T ; equilibrium values peak near 8000–10000 K and collapse once the gas ionises
- Each 10× in pressure shifts the peak about 1500 K higher
- Electrons diffuse 100× faster than heavy species; ions the slowest
- Wright collision integrals, Wilke mixing

Effective species diffusion D_s , m²/s, 1 atm (log)



Validation – Ramp shock interaction



Riemann solver test

- **Test case**
2D shock–ramp interaction, 1T, pure N_2
- **Initial condition**
Two uniform states (left and right) split by a discontinuity, as in a shock tube
- **Adaptive mesh**
Refinement follows the discontinuity and the ramp wall; the rest stays coarse

Validation – Ramp shock interaction



Pressure evolution

- **Incident shock**
The left-right discontinuity breaks up and the shock travels toward the ramp
- **Ramp interaction**
The shock hits the ramp and reflects, raising the pressure along the wall
- **What is verified**
The Riemann solver captures the shock without spurious oscillations at the EB wall

Combustion chamber in a shock tube – Mach number



Case setup

- **Chamber**
120 cm long, 20 cm diameter
- **Mixture**
He, H₂ and O₂ at molar fractions
He:H₂:O₂ = 8:2:1
- **Initial state**
5 bar, 300 K

Combustion chamber in a shock tube – Temperature and adaptive mesh

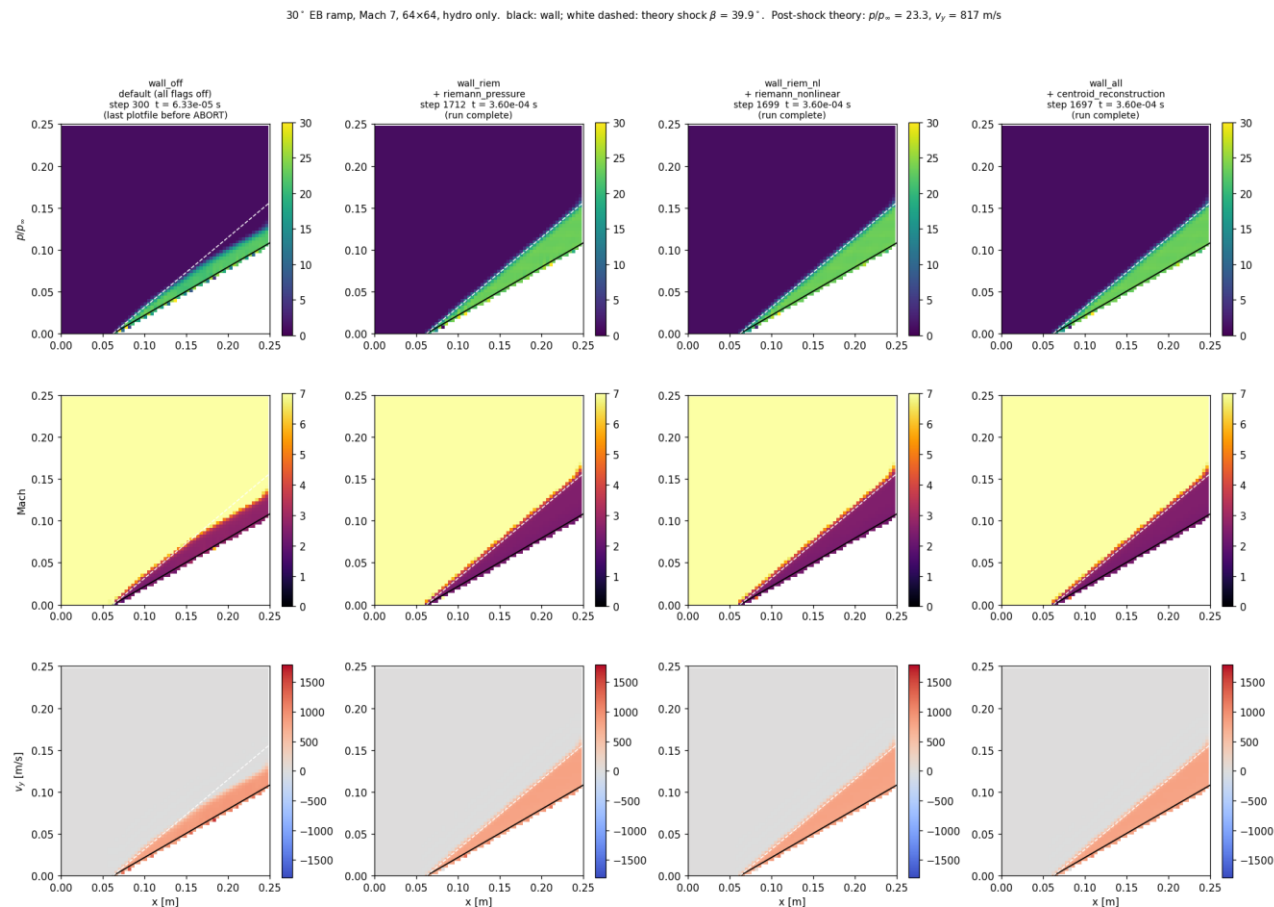


Numerical setup

- **Symmetry**
1/8 of the cylinder simulated, with 3 symmetry planes
- **Walls**
Curved wall and base, isothermal at 300 K
- **Kinetics and transport**
Davis H₂/O₂ mechanism, Eucken transport

30° ramp at Mach 7: the default wall treatment aborts at 63 μ s, while the Riemann wall flux runs to completion and puts the shock on the θ - β -M angle of 39.9°

2D Cartesian EB ramp, 64×64, hydro only. Rows: p/p_∞ , Mach, v_y . White dashed: theory, $\beta = 39.9^\circ$



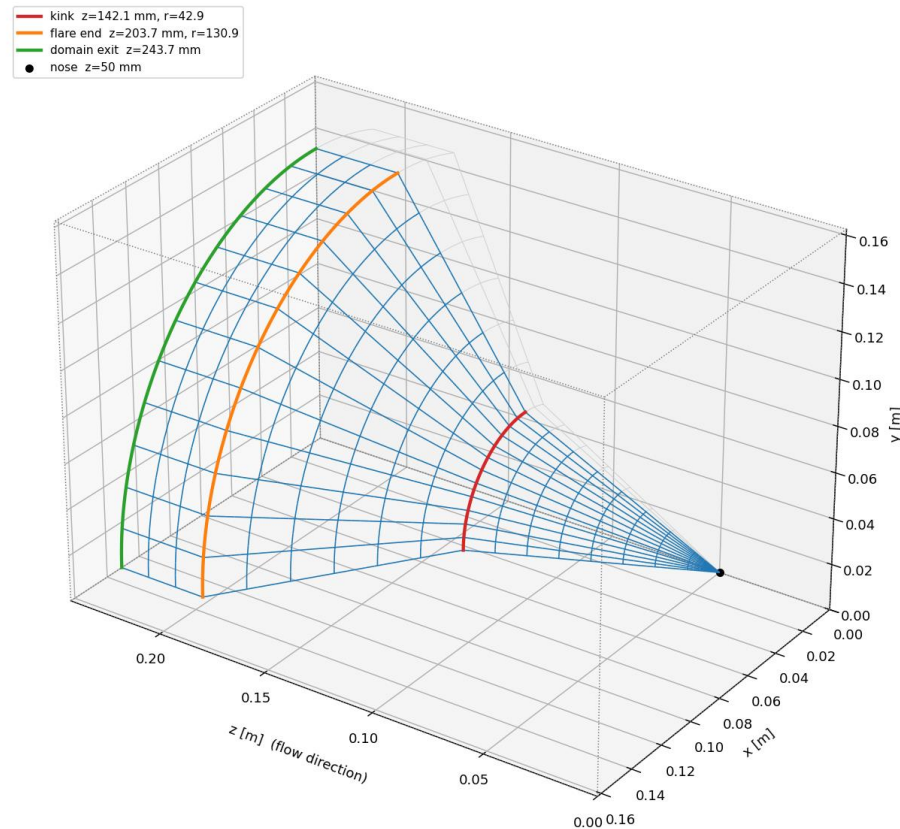
Four wall treatments

- **Default Flag: ABORT**
Last plotfile at step 300, $t = 63 \mu$ s;
shock lags theory and the post-shock layer is noisy at the wall
- **Riemann pressure: stable**
Runs to 360 μ s; shock sits on $\beta = 39.9^\circ$ and the post-shock band is uniform
- **Nonlinear Riemann, centroid**
No visible change on 64×64: same shock angle and post-shock state
- **Post-shock theory**
 $p/p_\infty = 23.3$ and $v_y = 817$ m/s;
the green band and orange v_y band match

Double cone geometry: the LENS 25°/55° body is an EB conical biramp, and only a quarter of it is simulated using two symmetry planes

Blue: EB surface inside the quarter domain ($x, y \geq 0$);

LENS XX double cone 25/55 deg - conical_biramp EB surface
blue = surface inside the quarter domain ($x, y \geq 0$); grey = continuation past the symmetry plane; dotted = domain box



Key stations along z

- **Nose**
 $z = 50$ mm, sharp tip on the axis
- **Kink, 25° → 55°**
 $z = 142.1$ mm, $r = 42.9$ mm
- **Flare end**
 $z = 203.7$ mm, $r = 130.9$ mm
- **Domain exit**
 $z = 243.7$ mm, outflow boundary

Upstream conditions

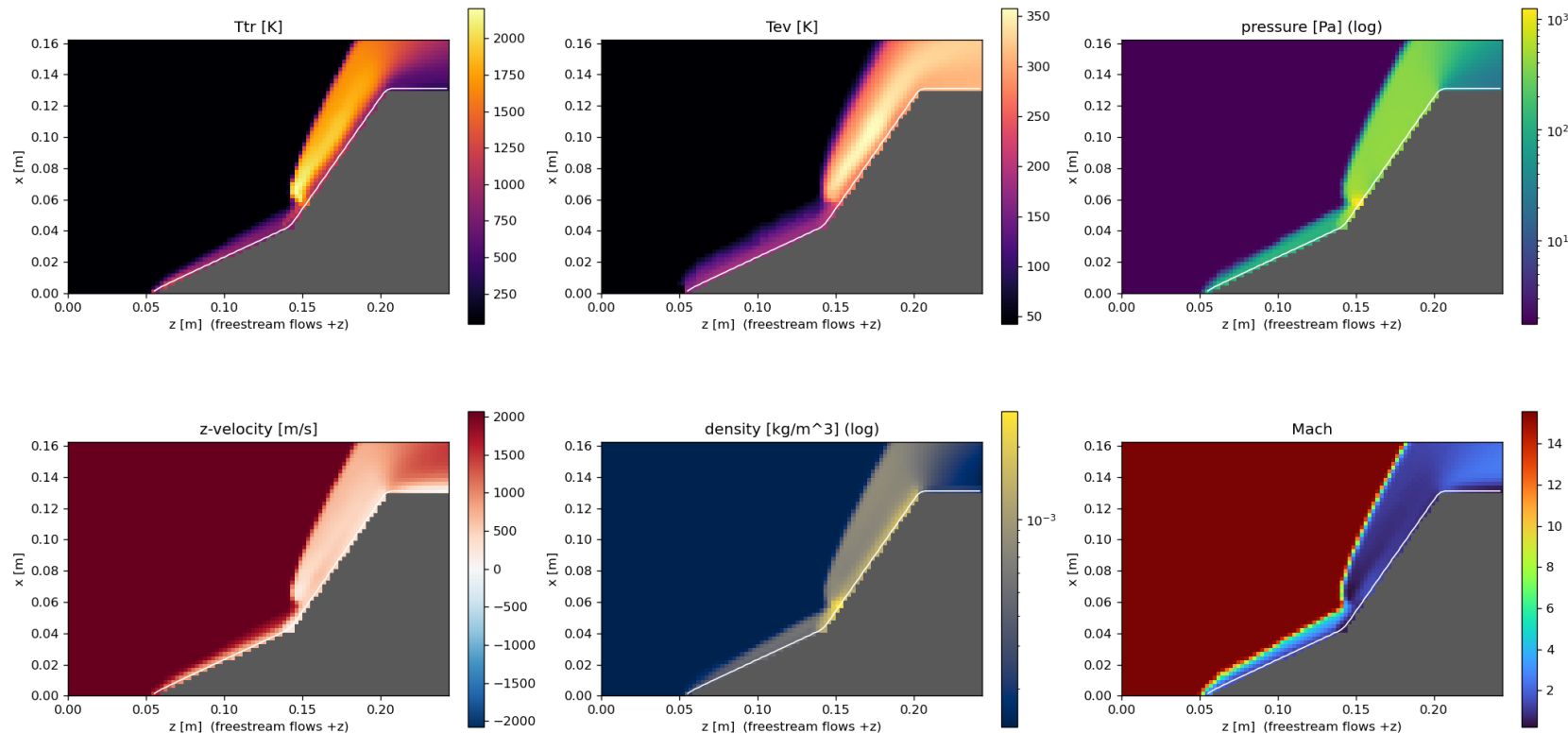
CUBRC/Holden LENS-I Run 7, pure N_2

ρ_∞	1.3955×10^{-4} kg/m ³
u_∞	2072.6 m/s along + z
$T_{tr} = T_{ev}$	42.61 K, equilibrium
Mixture	N_2 , mass fraction 1.0

Double cone geometry: the LENS 25°/55°

Symmetry plane $y = 0$ at $t = 441 \mu\text{s}$: translational and vibrational temperature, pressure, axial

Double cone (25/55 deg), N₂, 3D Cartesian quarter, 64x64x96, StateRedist sv=1e-3 — plt64_01000, $t = 4.409\text{e-}04 \text{ s}$ — symmetry plane $y=0$

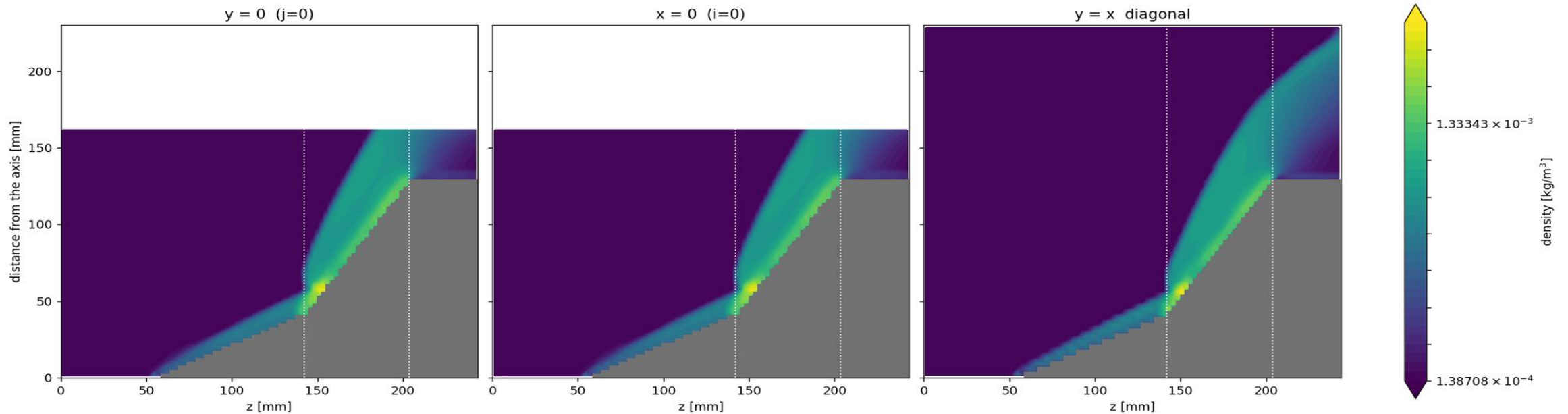


Case set-up

- **25°/55° double cone**
LENS geometry, kink at $z = 0.142 \text{ m}$
- **3D Cartesian quarter**
 $32 \times 32 \times 48$ base grid, $\Delta x = 5.08 \text{ mm}$, one AMR level
- **Two energy pools**
 T_{tr} and T_{ve} , N₂ mechanism
- **Cut-cell hydro**
StateRedist, small-volume threshold 10^{-3}
- **Freestream Mach ≈ 14**
cold isothermal wall

Double cone density: three meridional planes of one run

Single-level uniform $64 \times 64 \times 96$ grid at $t = 441 \mu\text{s}$: planes $y = 0$, $x = 0$ and the $y = x$ diagonal



Same flow, three cuts

The body is axisymmetric, so all three panels should match

White is outside the domain

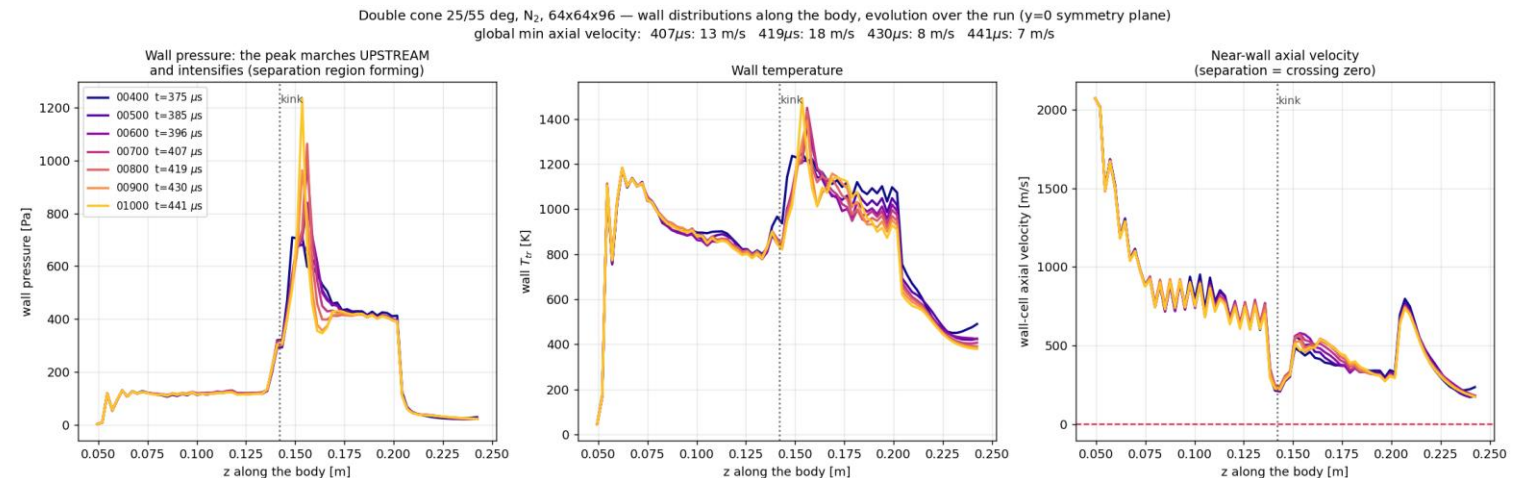
The diagonal plane reaches farther from the axis, $\sqrt{2} \times$ the box half-width

Along the wall, the pressure peak marches upstream and doubles to 1.2 kPa as separation forms, but near-wall velocity never crosses zero

Along the wall

Wall distributions on the $y = 0$ plane, seven snapshots from $t = 375$ to $441 \mu\text{s}$

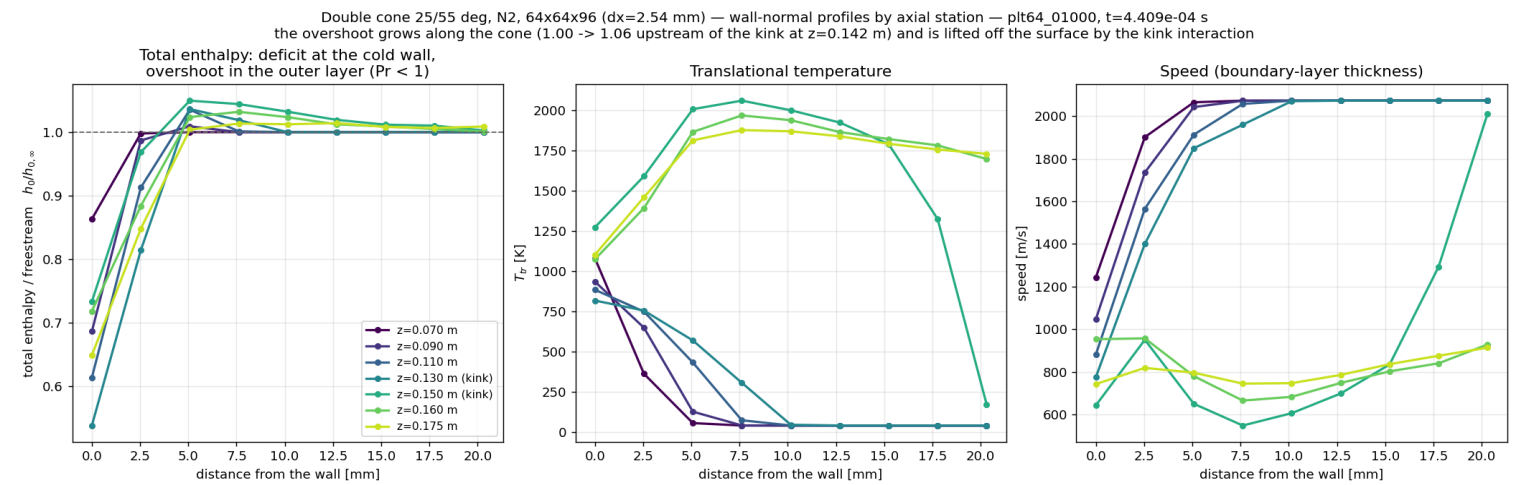
Kink at $z = 0.142 \text{ m}$



Away from the wall, at $t = 441 \mu\text{s}$

Wall-normal profiles at seven axial stations, $z = 0.070$ to 0.175 m , from the wall to 20 mm

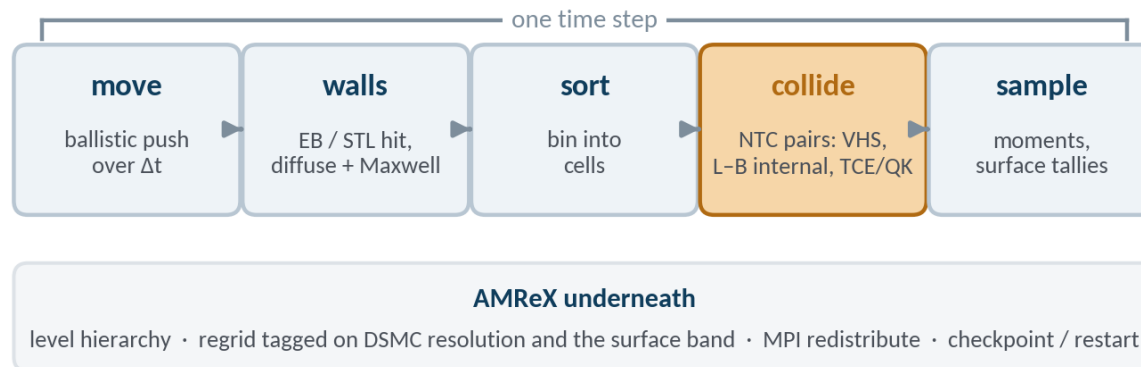
plt64_01000, $dx = 2.54 \text{ mm}$



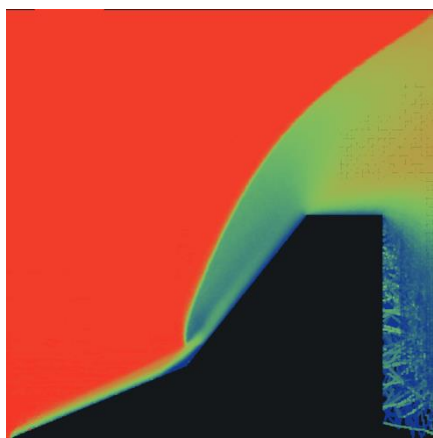
Prometheus — DSMC on AMReX

A direct simulation Monte Carlo solver for rarefied and transitional flow, built on the same backbone as HelioS.

The DSMC cycle, on an AMR hierarchy



CUBRC Run 7 — 25°/55° double cone, N₂



110 × 125 base grid, 3 levels, ratio 2
228 820 active leaf cells, 914 162 particles
 $\Delta t = 0.12 \mu s$, 41 084 steps, 4.93 ms
N₂, VHS, $u_\infty = 2073 \text{ m/s}$, $T_{v,\infty} = 1986 \text{ K}$
axisymmetric r-z, EB revolved profile, 8 MPI ranks

In the collision cell

NTC pair selection with hard-sphere, VHS or VSS cross sections. Larsen–Borgnakke rotational exchange and quantised harmonic-oscillator vibration, mode resolved. Finite-rate chemistry by TCE and QK.

Geometry, mesh, data

STL bodies through AMReX EB2; diffuse thermal walls with Maxwell accommodation and surface tallies. Cartesian mesh, adaptive refinement, MPI decomposition.

How it is checked

29 validation tests against analytic results: collision rates, equipartition, chemistry kinetics, free-molecular and diffuse-wall fluxes, Rankine–Hugoniot. Seven production-gate decks compare frozen collision and sampling digests, so any change that perturbs a trajectory is caught.

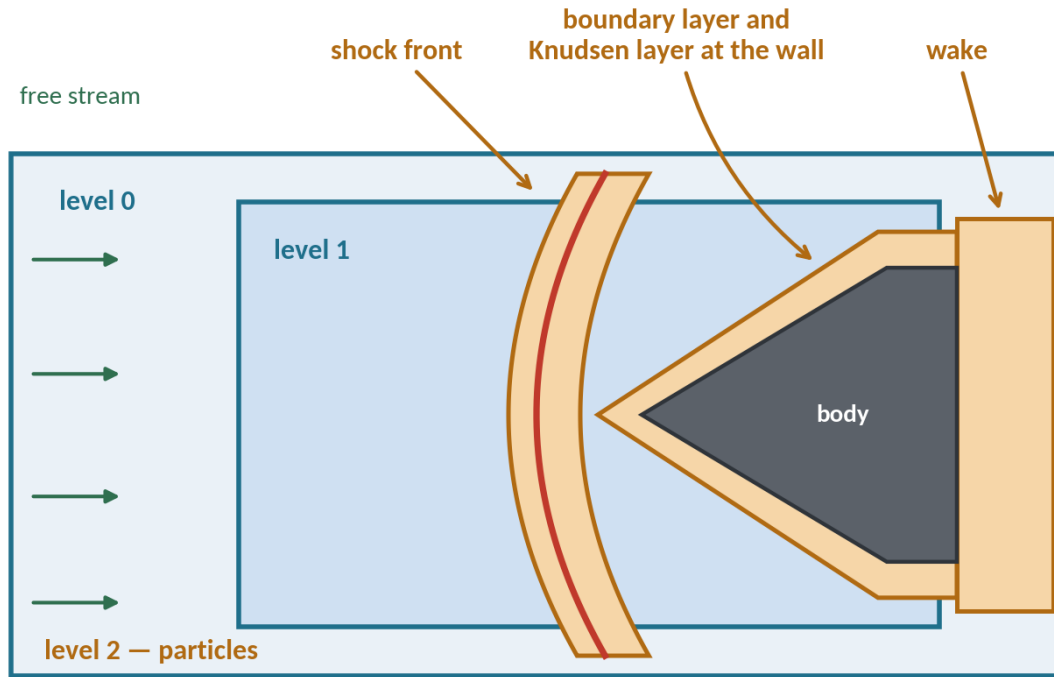
Run 7: where it stands

Wall pressure within 16 % MAPE of the digitised experiment; heat flux still 61 %, about twofold high on the cone and at reattachment.

One backbone, two solvers: the CFD–DSMC hybrid

HelioS and Prometheus are already AMReX applications over the same boxes, levels and EB geometry, the hybrid is a coupling problem, not a rewrite.

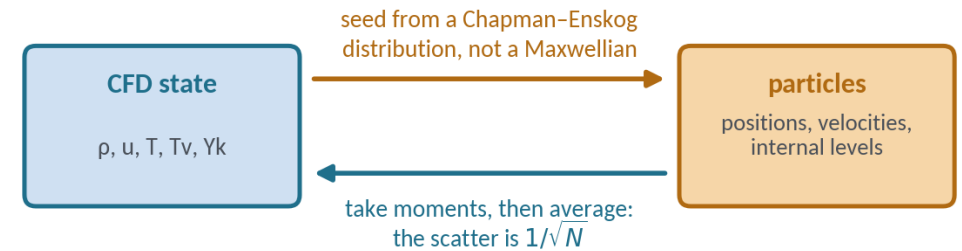
Levels as solver regions



Levels 0–1 continuum (HelioS); particles on the shock, the wall and the wake.

What is already shared

The same Box, BoxArray and DistributionMap, level hierarchy and subcycling, EB geometry from the same STL, plotfile and checkpoint format. The coupling can live in memory, no file exchange, no second mesh.



The catch, and the prize

The wall band is the costly one: λ is smallest where the gas is densest, so particles are dearest exactly where the heating is measured. In exchange the cut cells become interior to the particle region, the wall boundary condition and the small-cell problem both move to DSMC.

Future work and Summary

Key points

01 One solver, several models

Multi-species Navier–Stokes with one equation per energy pool; 1T, 2T, 3T and 4T are the same code with a different pool model.

02 Stiffness isolated by the split

S–D–H–D–S: explicit Godunov for hydro only, implicit backward Euler for diffusion, CVODE per cell for the sources.

03 Cut cells instead of body-fitted meshes

EB with state redistribution, and non-linear Riemann Wall treatment.

04 AMR that respects the operator

Hyperbolic subcycled, implicit operators on one common timestep: 6 diffusion solves per coarse step instead of 14.

05 Verified before it is used

Physics validated: SPARK database and literature

Where it goes next

● Finish the GPU port

Thermodynamics and transport are still mostly host-side

● Double cone to steady separation

The wall pressure peak is still marching upstream at $441 \mu\text{s}$

● Couple SPARK line-by-line radiation

The radiative pool term is in the equations, not yet in the runs. But implementation possible by using MLMG AMReX solvers.

● State-to-state kinetics

STS model is a model file for physics, not a rewrite of numerical solver

● Close the CFD–DSMC hybrid

Kn switching and Chapman–Enskog seeding.

