There and Back Again: A heat transfer tale

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21 April 2022

Talk Outline

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0   Setting the scene
I   Status of the code project
II  Thermochemistry development
III Steady-state accelerator development
IV  Concluding remarks
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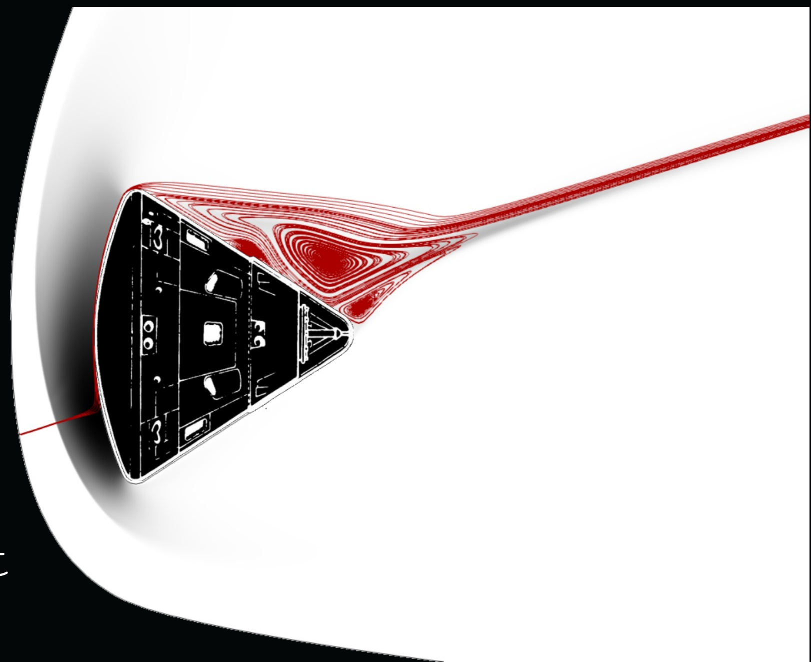
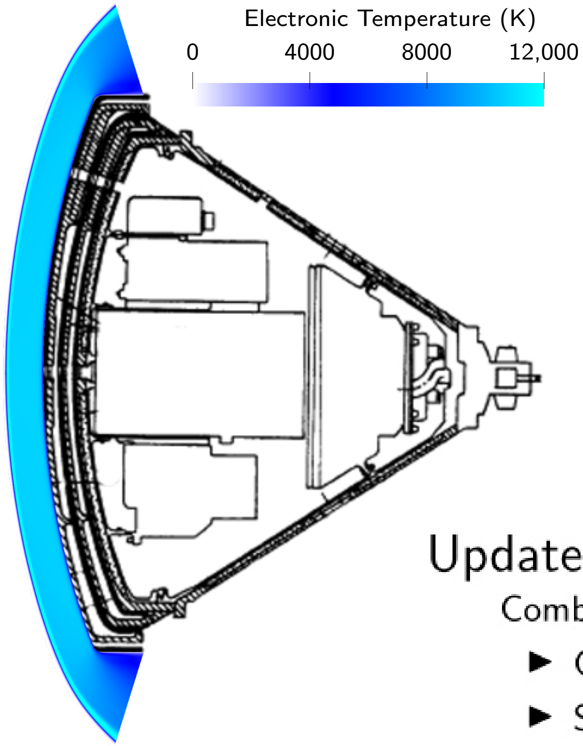


0. Setting the scene

Update: Simulations of Fire II

Fire II flight test from 1965 is a difficult benchmark problem

- v= 11km/s, altitude 71 km, capsule size $\approx 1m$
- Lightly radiating ($\approx 10\%$ of the heat load)
- Measurements of total and radiation heat transfer



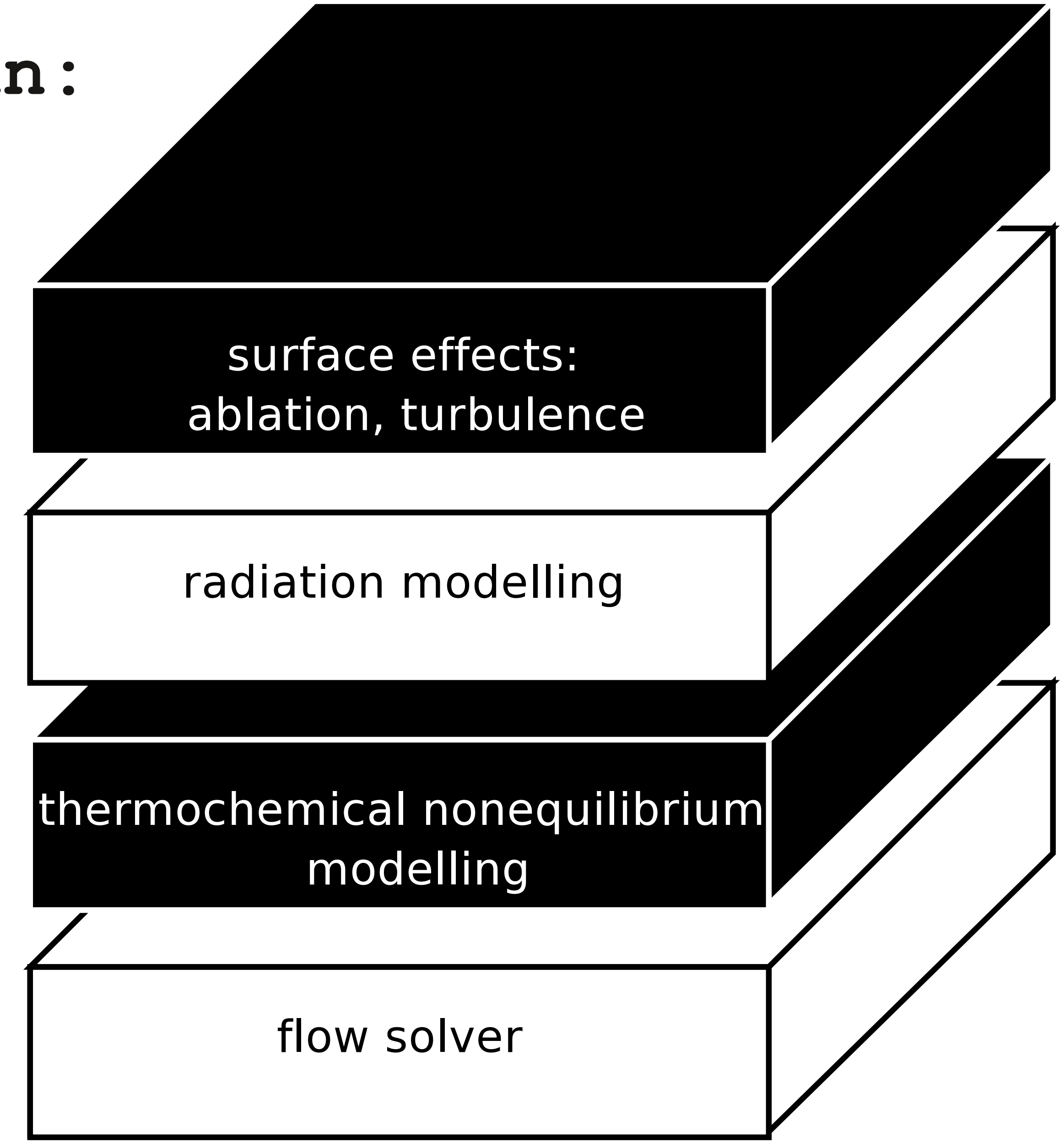
Update: Simulations of Fire II

Combination of all these fixes, + improvements to the NK solver

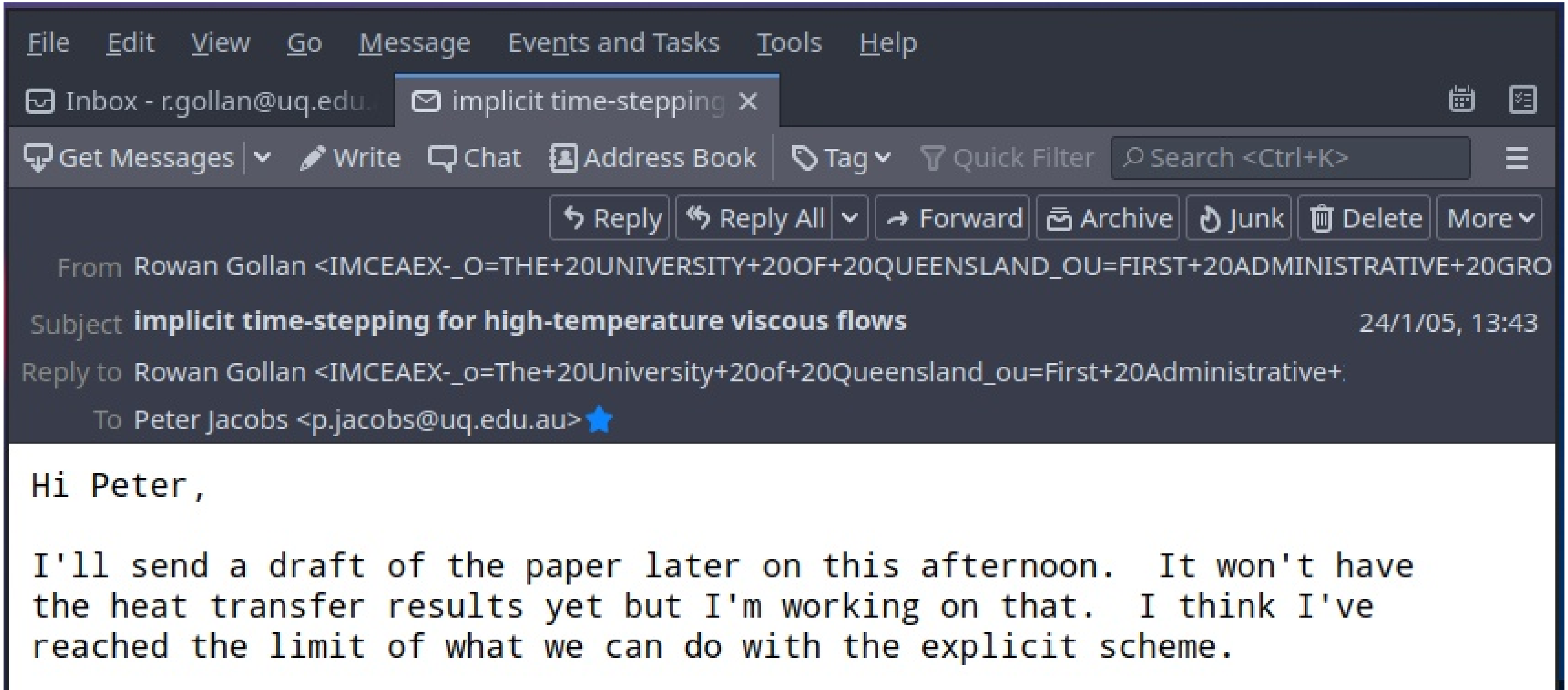
- GridPro grid with 100x257 elements, first cell $2\mu m$
- Simulations converge in ≈ 75 minutes, on 16 cores
- Reasonable agreement with flight data
- Good agreement to Hash et al. AIAA paper 2007-605

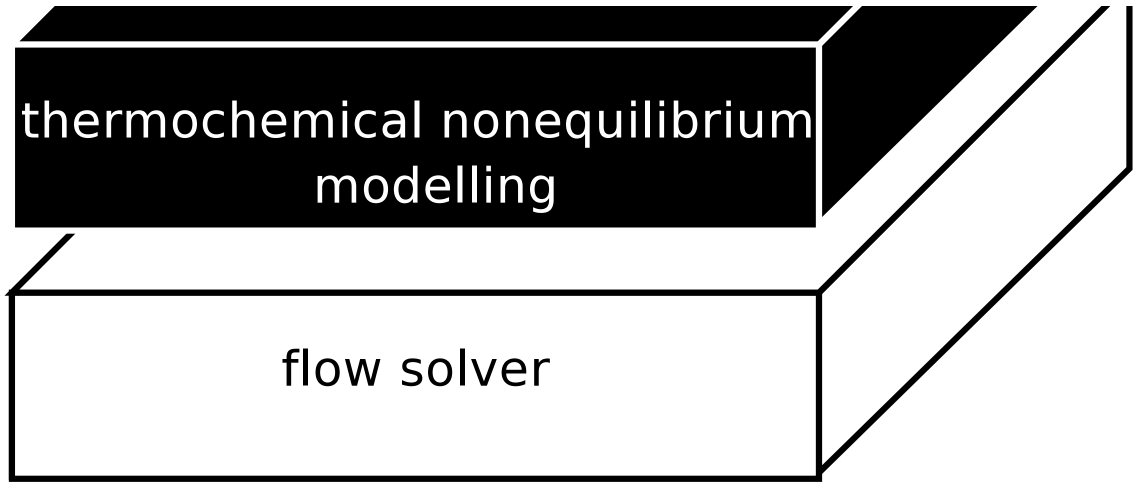
Where the journey began...

Thesis plan:

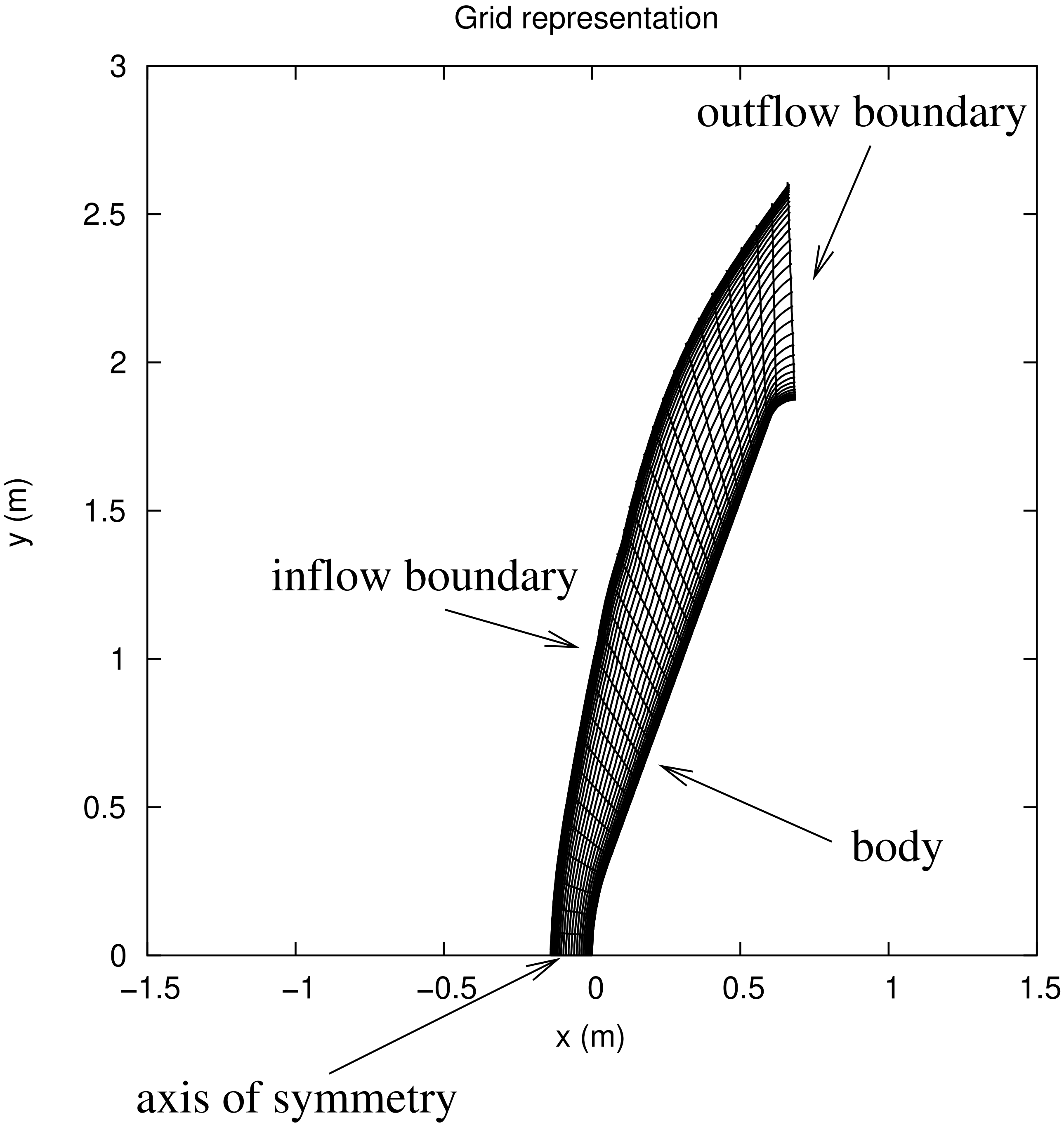


Where it ended

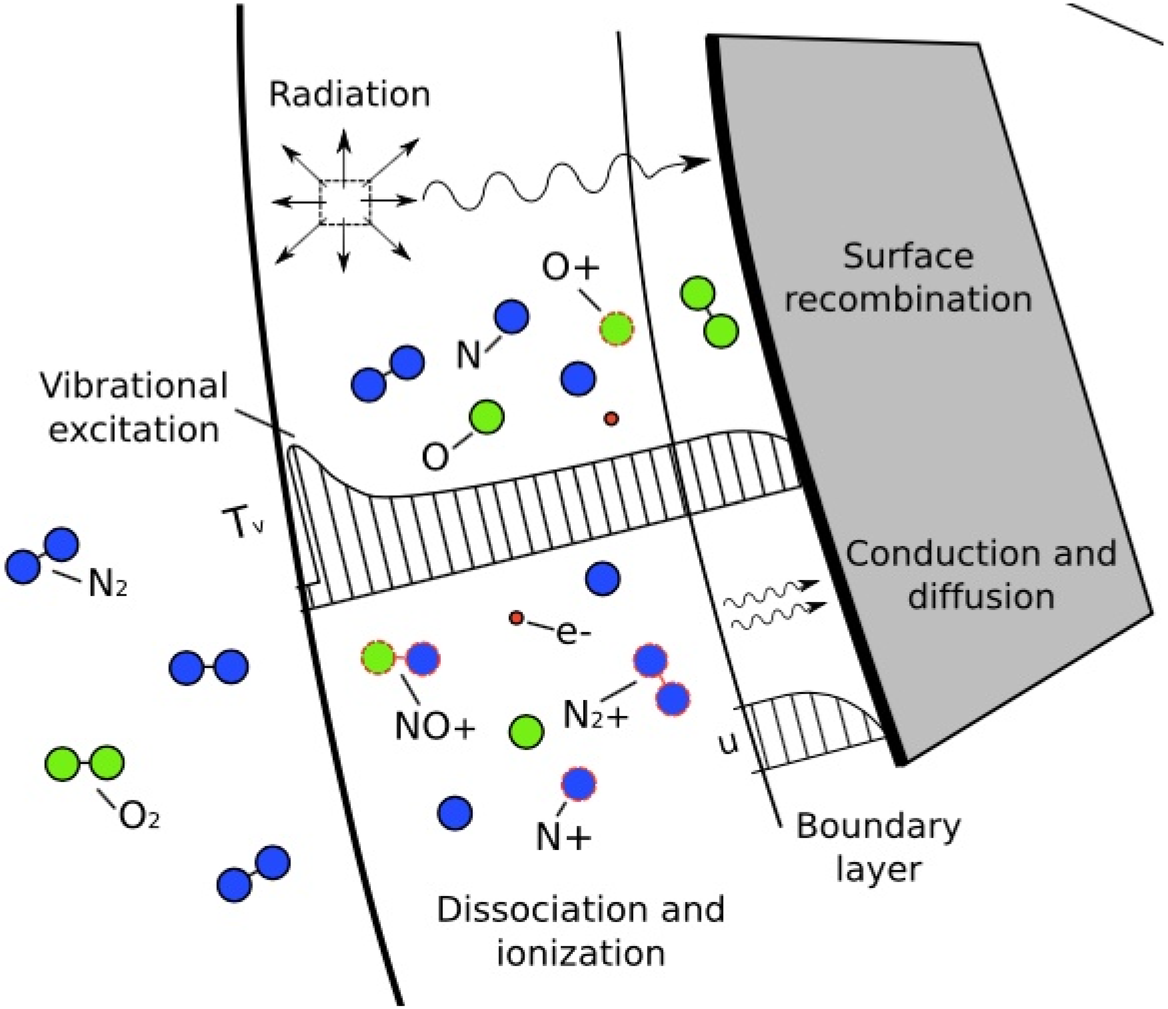




Where it ended



The hypersonic blunt body flowfield



Required modelling/technologies

+ shock-fitting
+ high-quality grid generation
+ accelerator for steady-state
+ nonequilibrium (multi-temperature) thermodynamics
+ nonequilibrium transport properties
+ wall-catalytic boundary conditions
+ finite-rate chemistry (w multi-T effects)
+ energy exchange mechanisms
+ turbulence modelling
+ surface ablation
+ coupling to radiation field
+ coupling to magnetohydrodynamic effects

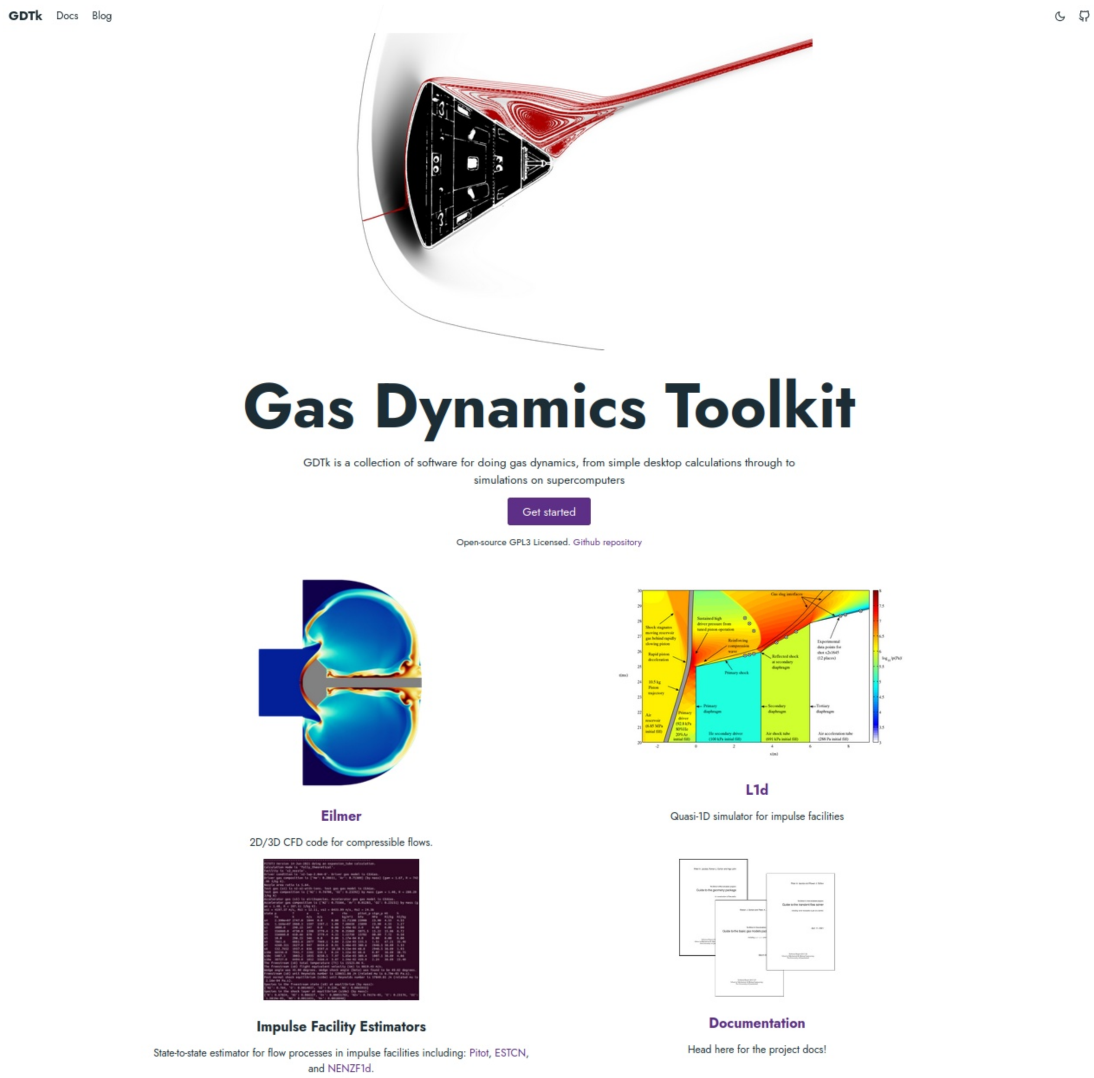
Thanks: Daniel Potter

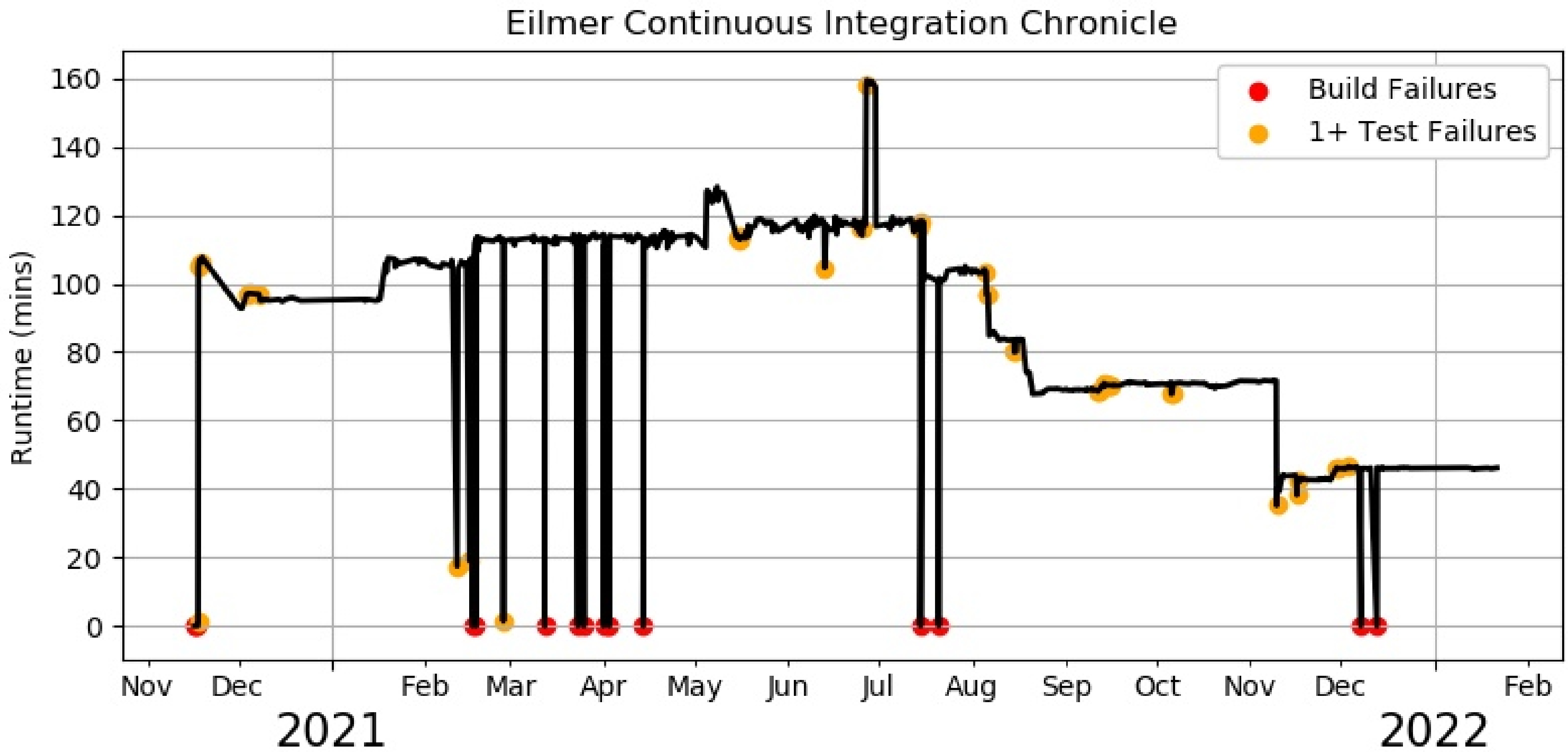
I: Status of the code project -- GDTk

+ core dev team increased from 2 to 4
+ increment in sophistication of development processes
+ continuous integration testing
+ restructure of repositories (code, website, docs)
+ moved to github for hosting

Supporting users

+ website
+ documentation:
  user guides, reference manuals,
  tech notes, catalogue of examples
+ issue tracker
+ Eilmer monthly meet-ups
+ email response to queries
+ face-to-face help
+ version releases





Eilmer Continuous Integration Chronicle
Build Failures
1+ Test Failures
Runtime (mins)
160
140
120
100
80
60
40
20
0
Nov
Dec
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec
Feb
2021
2022

II: Thermochemistry development

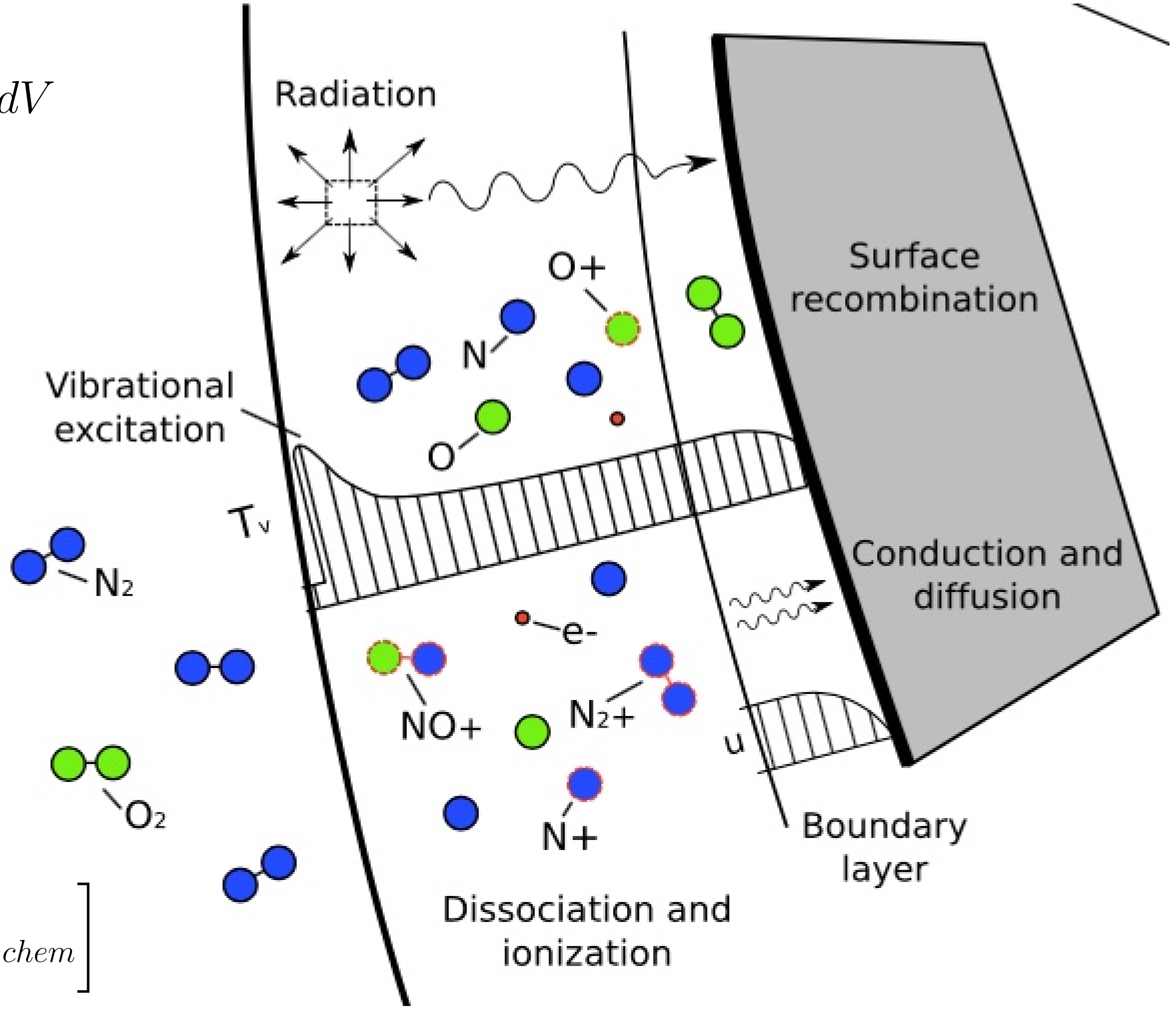
$$\frac{\partial}{\partial t}\int_V \mathbf{U}\, dV = -\oint_S (\mathbf{F}_c - \mathbf{F}_v)\cdot \hat{n}\, dA + \int_V \mathbf{Q}\, dV$$

$$\mathbf{U} = \begin{bmatrix} \vdots \\ \rho e_v \end{bmatrix}$$

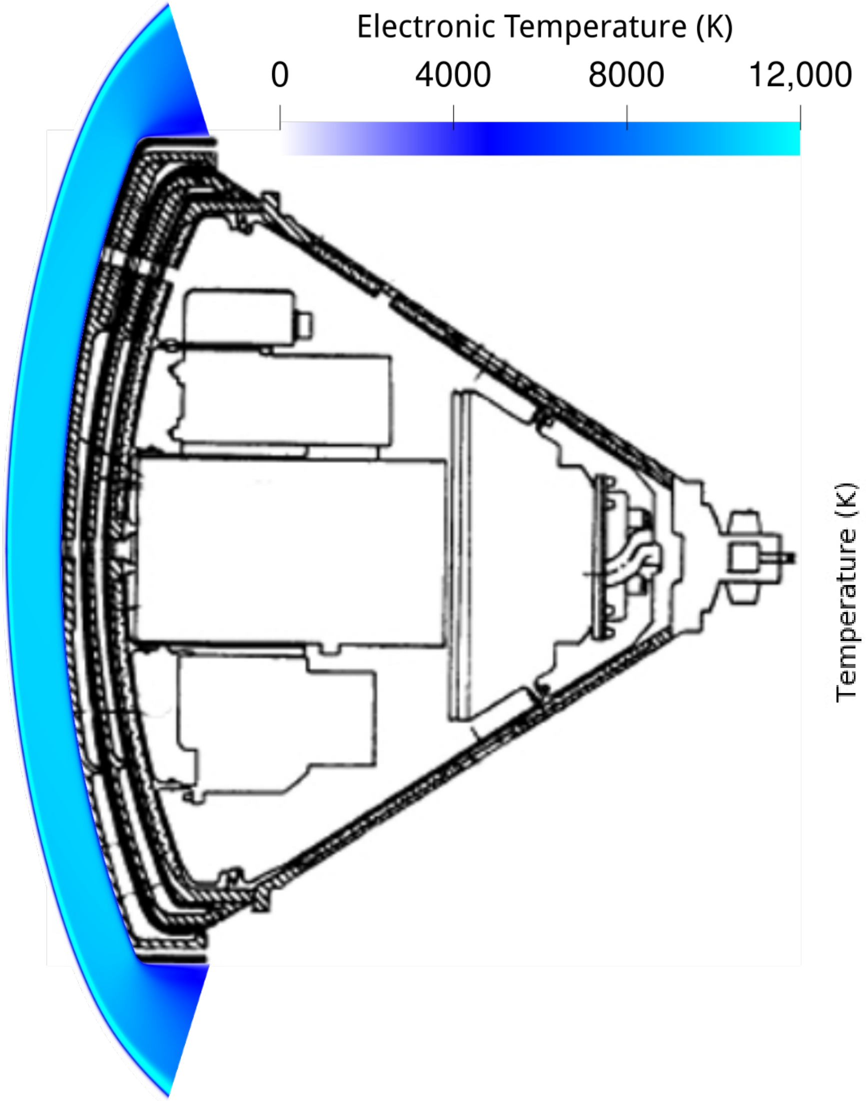
$$\mathbf{F}_i = \begin{bmatrix} \vdots \\ \rho e_v u \end{bmatrix}\hat{i} + \begin{bmatrix} \vdots \\ \rho e_v v \end{bmatrix}\hat{j} + \begin{bmatrix} \vdots \\ \rho e_v w \end{bmatrix}\hat{k}$$

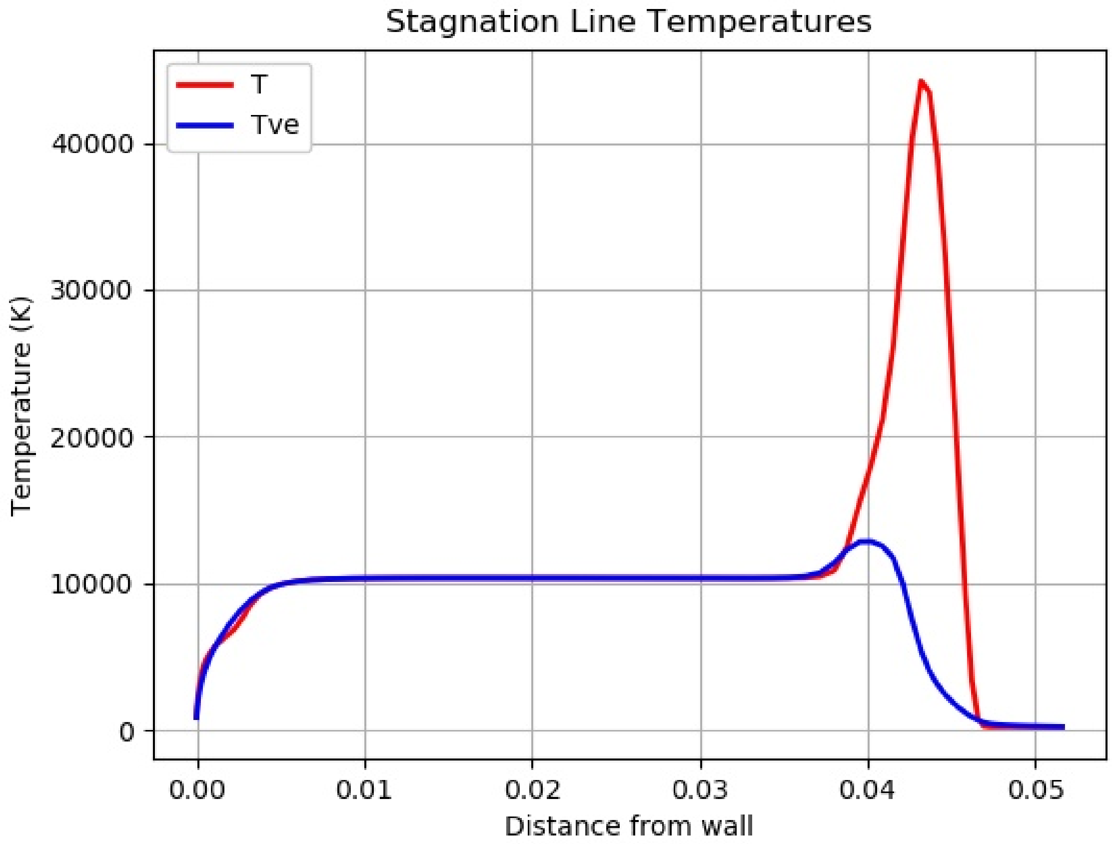
$$\mathbf{F}_v = \begin{bmatrix} \vdots \\ \kappa_v \frac{\partial T_v}{\partial x} - \sum_s \rho h_{vs} D_s \frac{\partial Y_s}{\partial x} \end{bmatrix}\hat{i} + \begin{bmatrix} \vdots \\ \kappa_v \frac{\partial T_v}{\partial y} - \sum_s \rho h_{vs} D_s \frac{\partial Y_s}{\partial y} \end{bmatrix}\hat{j} + \begin{bmatrix} \vdots \\ \kappa_v \frac{\partial T_v}{\partial z} - \sum_s \rho h_{vs} D_s \frac{\partial Y_s}{\partial z} \end{bmatrix}\hat{k}$$

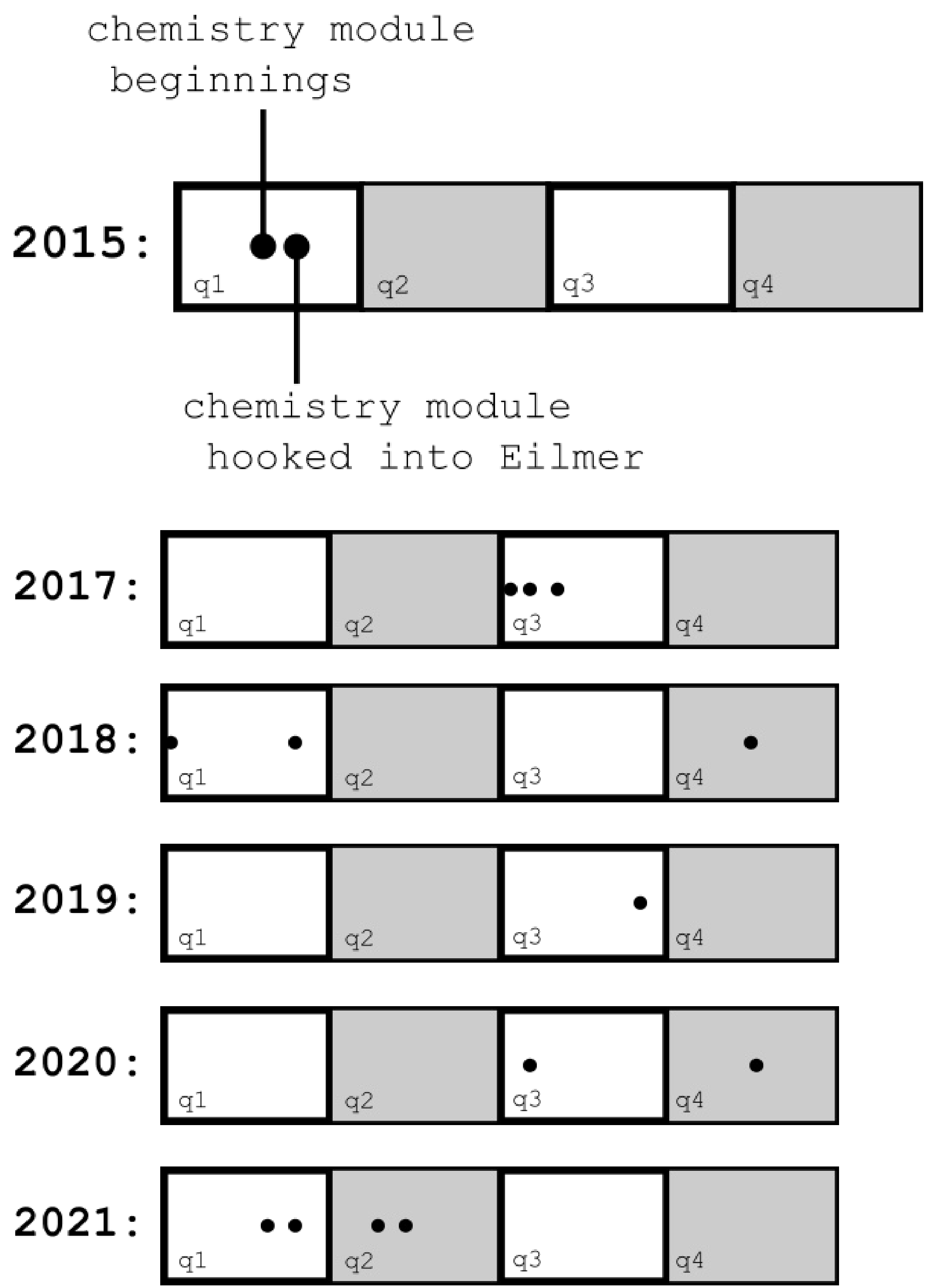
$$\mathbf{Q} = \begin{bmatrix} \vdots \\ \sum_s Q^{vib-trans} + \sum_s Q^{elec-trans} + \sum_r Q_r^{vib-chem} \end{bmatrix}$$

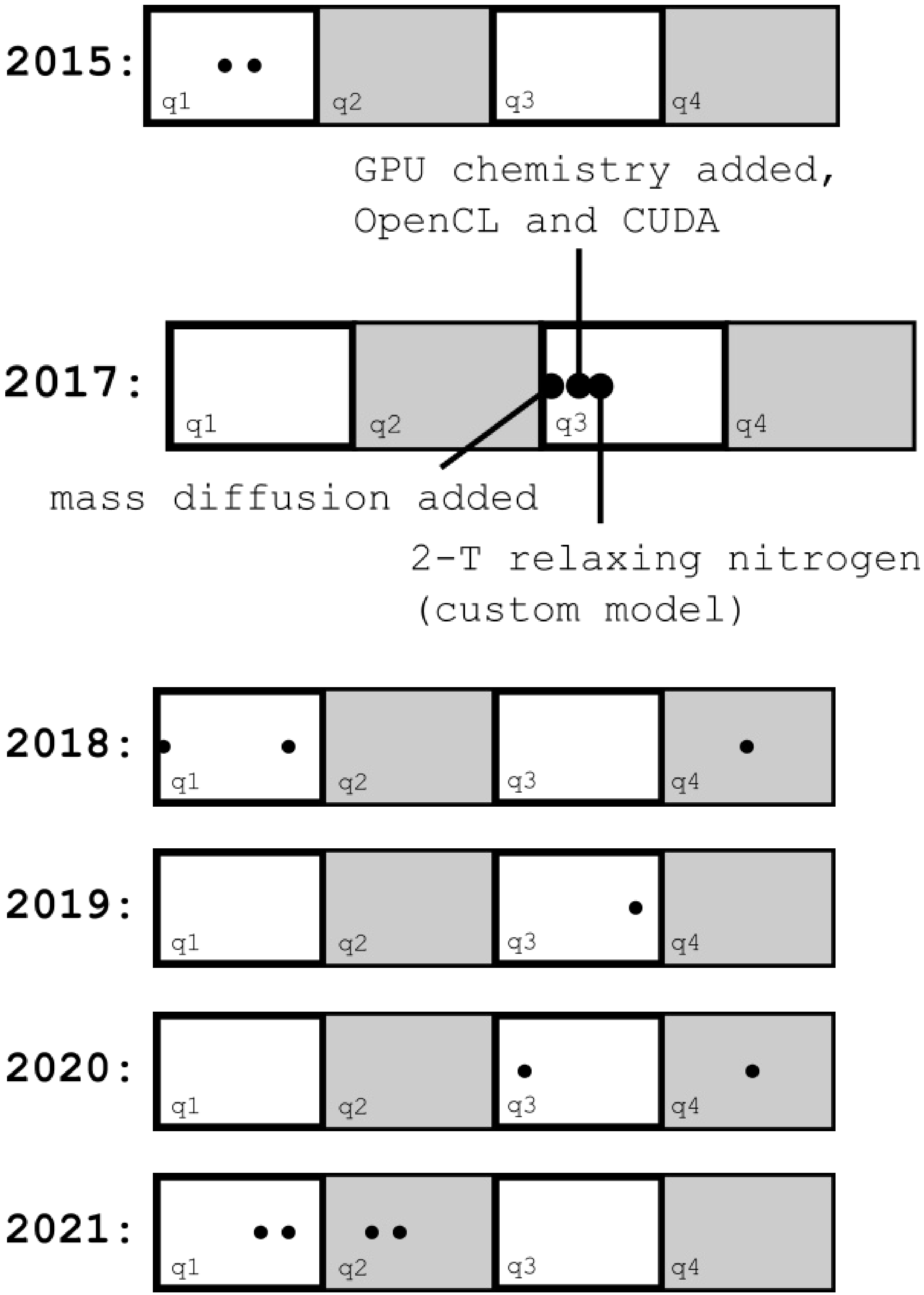


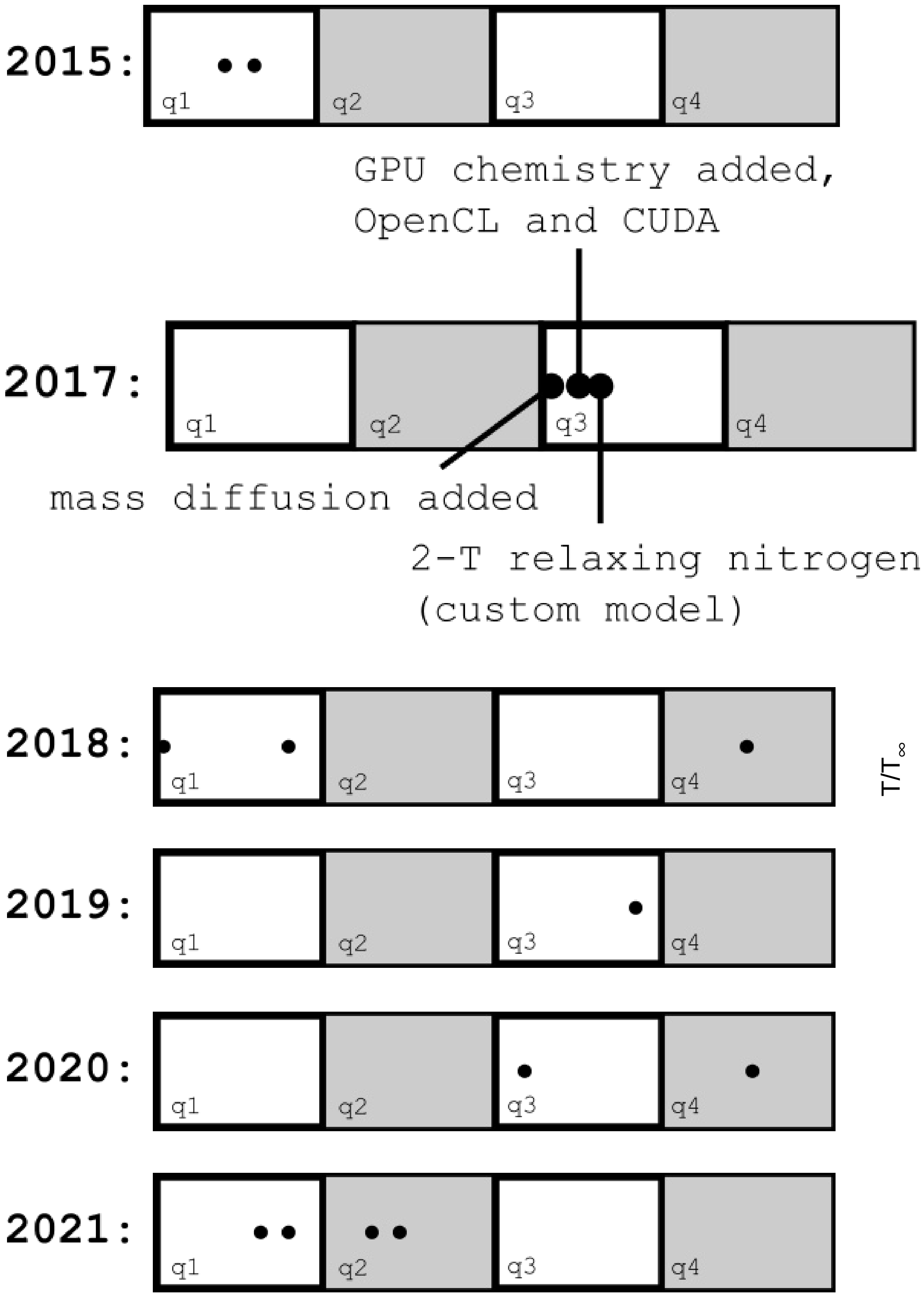
II: Thermochemistry development



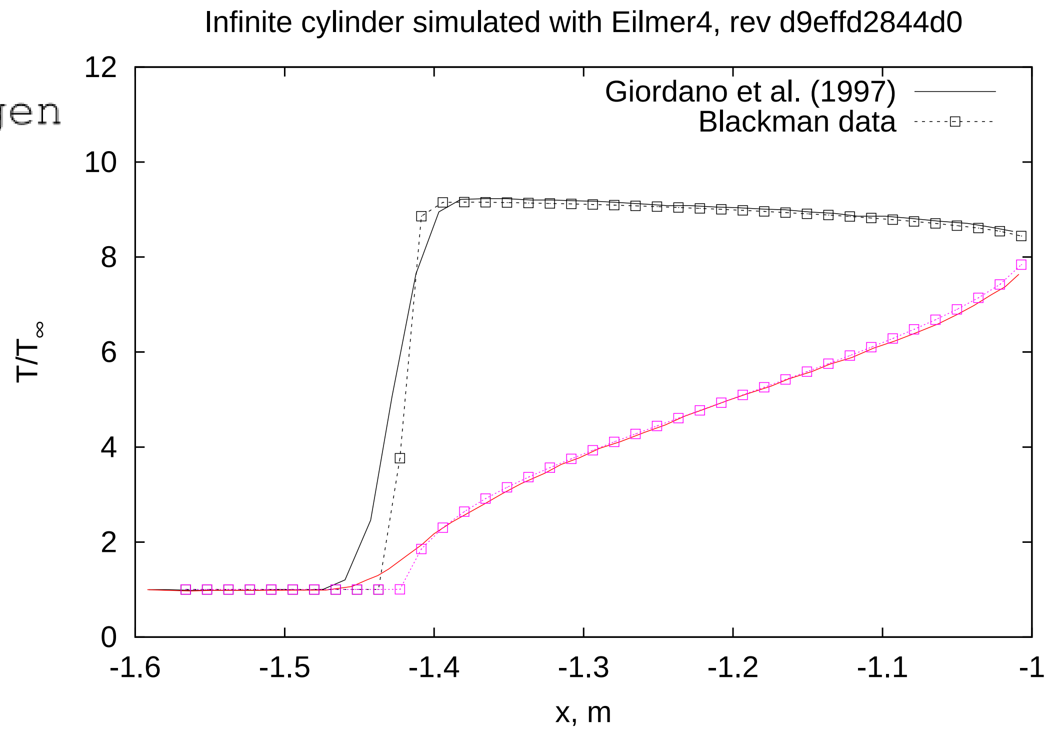



chemistry module
beginnings
2015:
q1
q2
q3
q4
chemistry module
hooked into Eilmer
2017:
2018:
2019:
2020:
2021:

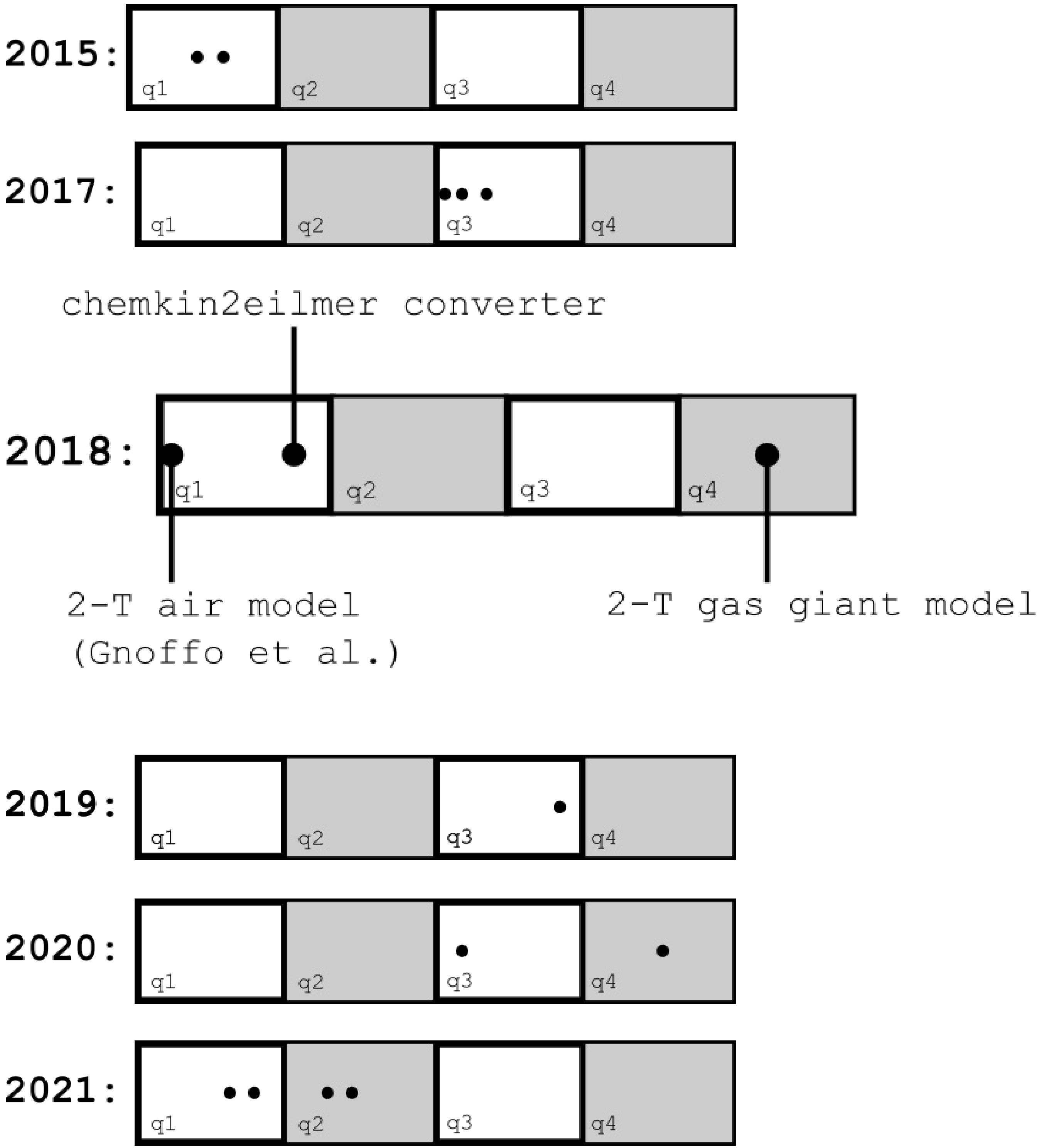

2015:
q1
q2
q3
q4
GPU chemistry added,
OpenCL and CUDA
2017:
q1
q2
q3
q4
mass diffusion added
2-T relaxing nitrogen
(custom model)
2018:
q1
q2
q3
q4
2019:
q1
q2
q3
q4
2020:
q1
q2
q3
q4
2021:
q1
q2
q3
q4



2015:
q1
q2
q3
q4
GPU chemistry added,
OpenCL and CUDA
2017:
q1
q2
q3
q4
mass diffusion added
2-T relaxing nitrogen
(custom model)
2018:
q1
q2
q3
q4
2019:
q1
q2
q3
q4
2020:
q1
q2
q3
q4
2021:
q1
q2
q3
q4



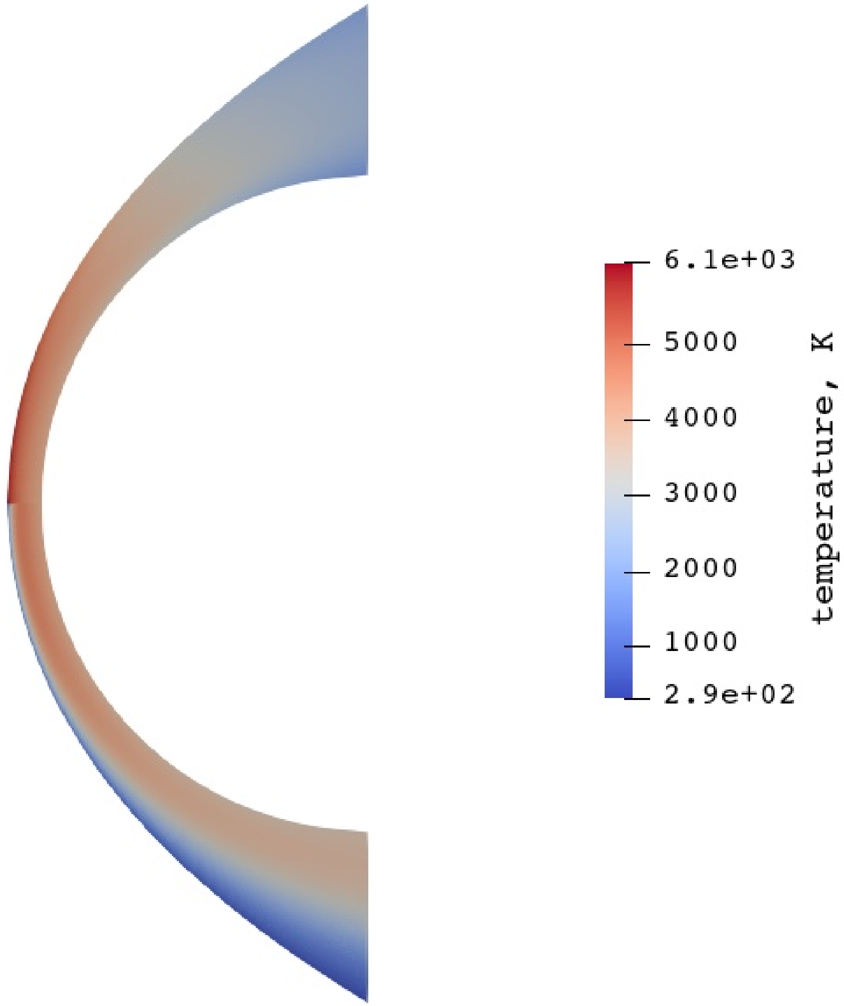
Infinite cylinder simulated with Eilmer4, rev d9effd2844d0
Giordano et al. (1997)
Blackman data
T/T_∞
x, m
0
2
4
6
8
10
12
-1.6
-1.5
-1.4
-1.3
-1.2
-1.1
-1


2015:
q1
q2
q3
q4
2017:
q1
q2
q3
q4
chemkin2eilmer converter
2018:
q1
q2
q3
q4
2-T air model
(Gnoffo et al.)
2-T gas giant model
2019:
q1
q2
q3
q4
2020:
q1
q2
q3
q4
2021:
q1
q2
q3
q4

```
! Chemkin-style input file
! Prepared by: Rowan J. Gollan
! Date: 2017-09-23
!
! This is an example to test out the chemkin2eilmer converter.

ELEMENTS
N
END

SPECIES
N2 N
END

REACTIONS
N2 + N2 <=> N + N + N2       7.00e21  -1.6    224951.04
                        REV/ 1.09e16  -0.5    0.0       /
N2 + N <=> N + N + N         3.00e22  -1.6    224951.04
                        REV/ 2.32e21  -1.5    0.0       /
END
```

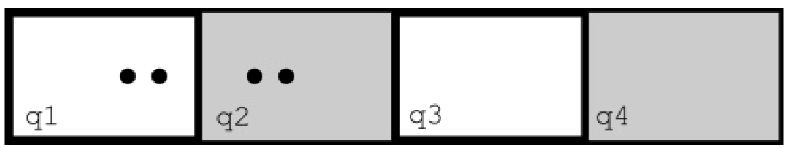
```
-- Auto-generated by chemkin2eilmer on: 20-Apr-2022 21:28:28

Config{
   odeStep = {method='alpha-qss'}
}
Reaction{
        'N2 + N2 <=> N + N + N2',
        fr={'Arrhenius', A=7.000000e+21, n=-1.600000e+00, C=1.132000e+05},
        br={'Arrhenius', A=1.090000e+16, n=-5.000000e-01, C=0.000000e+00},
}

Reaction{
        'N2 + N <=> N + N + N',
        fr={'Arrhenius', A=3.000000e+22, n=-1.600000e+00, C=1.132000e+05},
        br={'Arrhenius', A=2.320000e+21, n=-1.500000e+00, C=0.000000e+00},
}
```

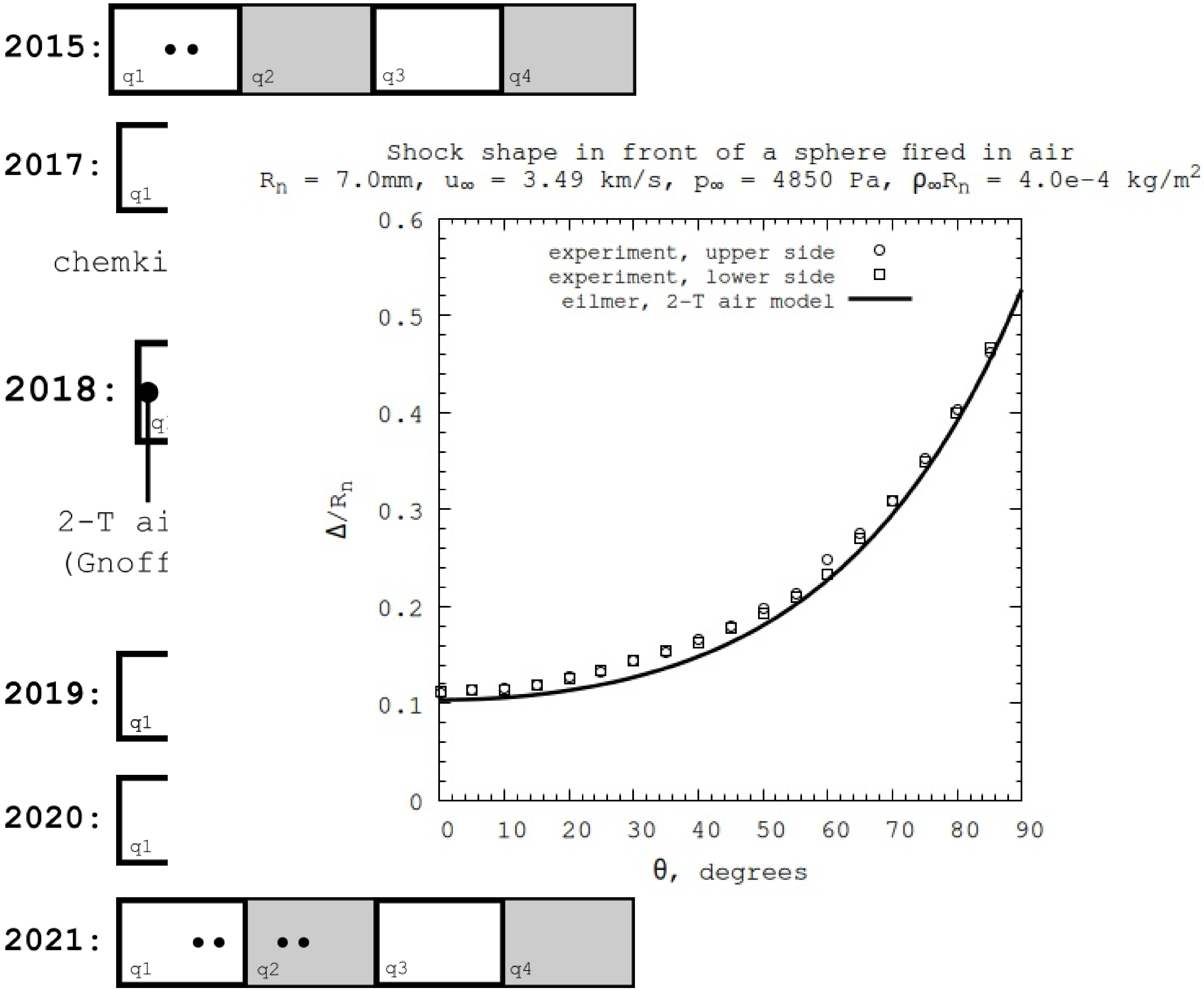
top half: transrotational temperature



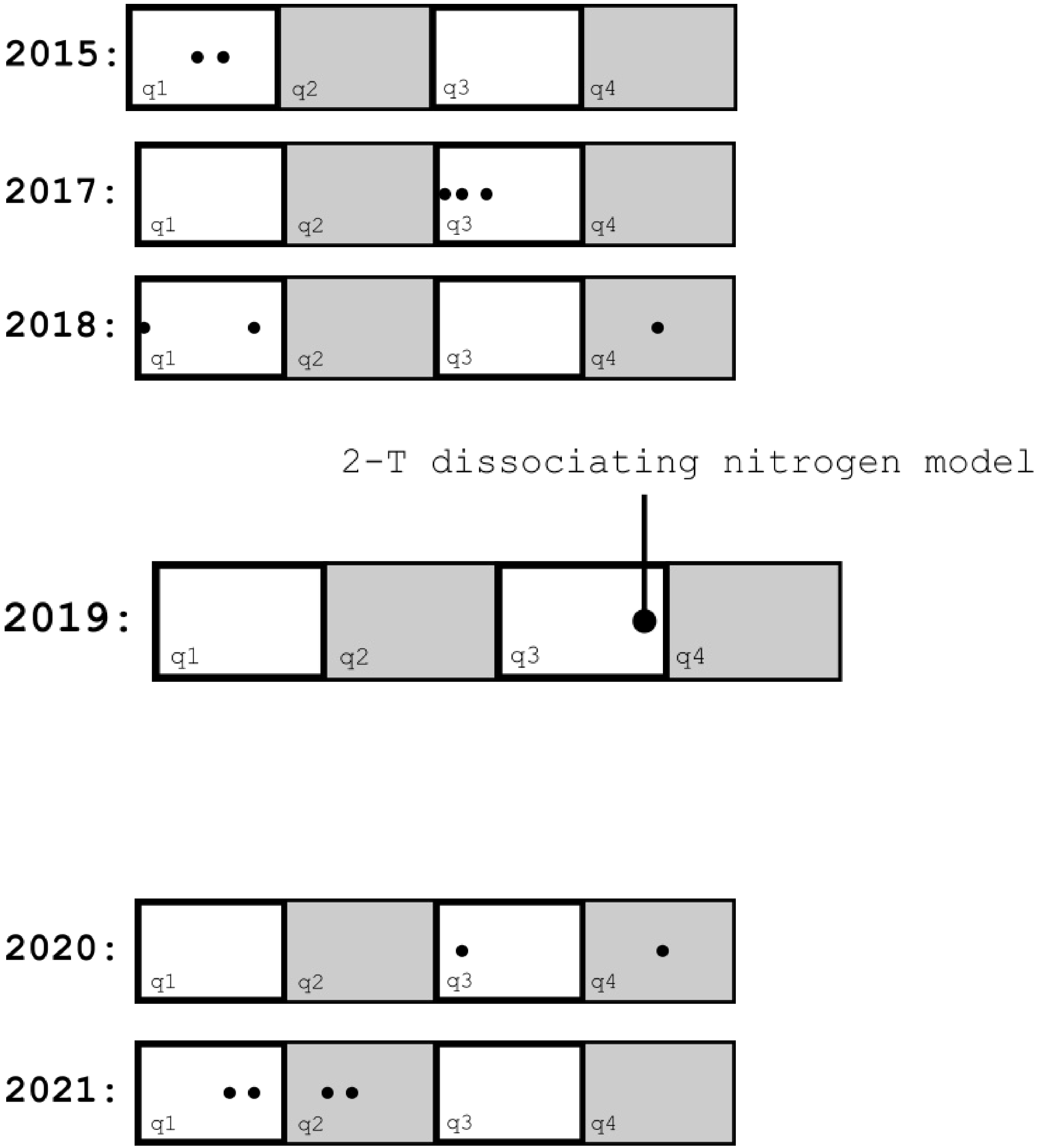
bottom half: vibroelectronic temperature

2021:

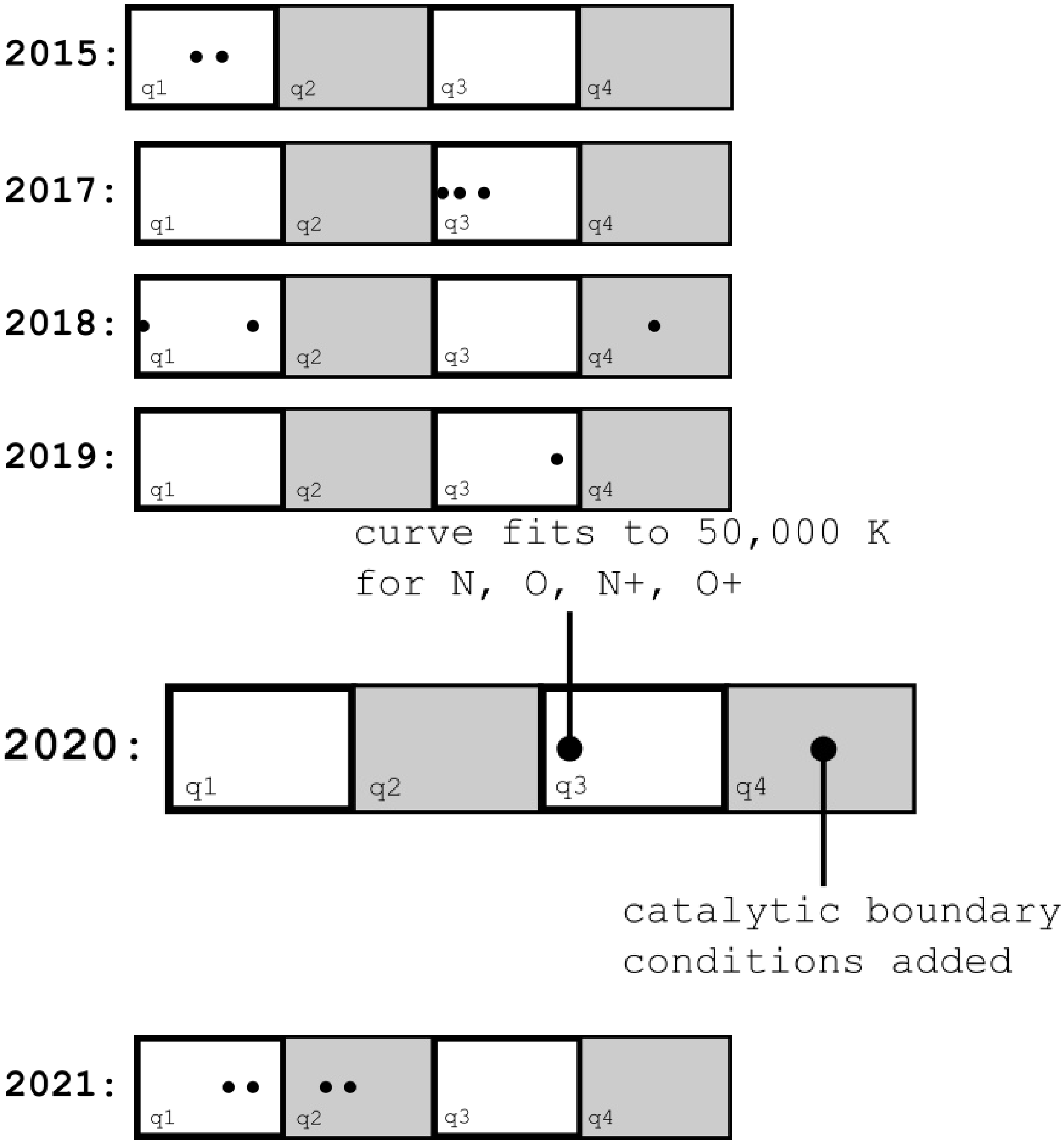


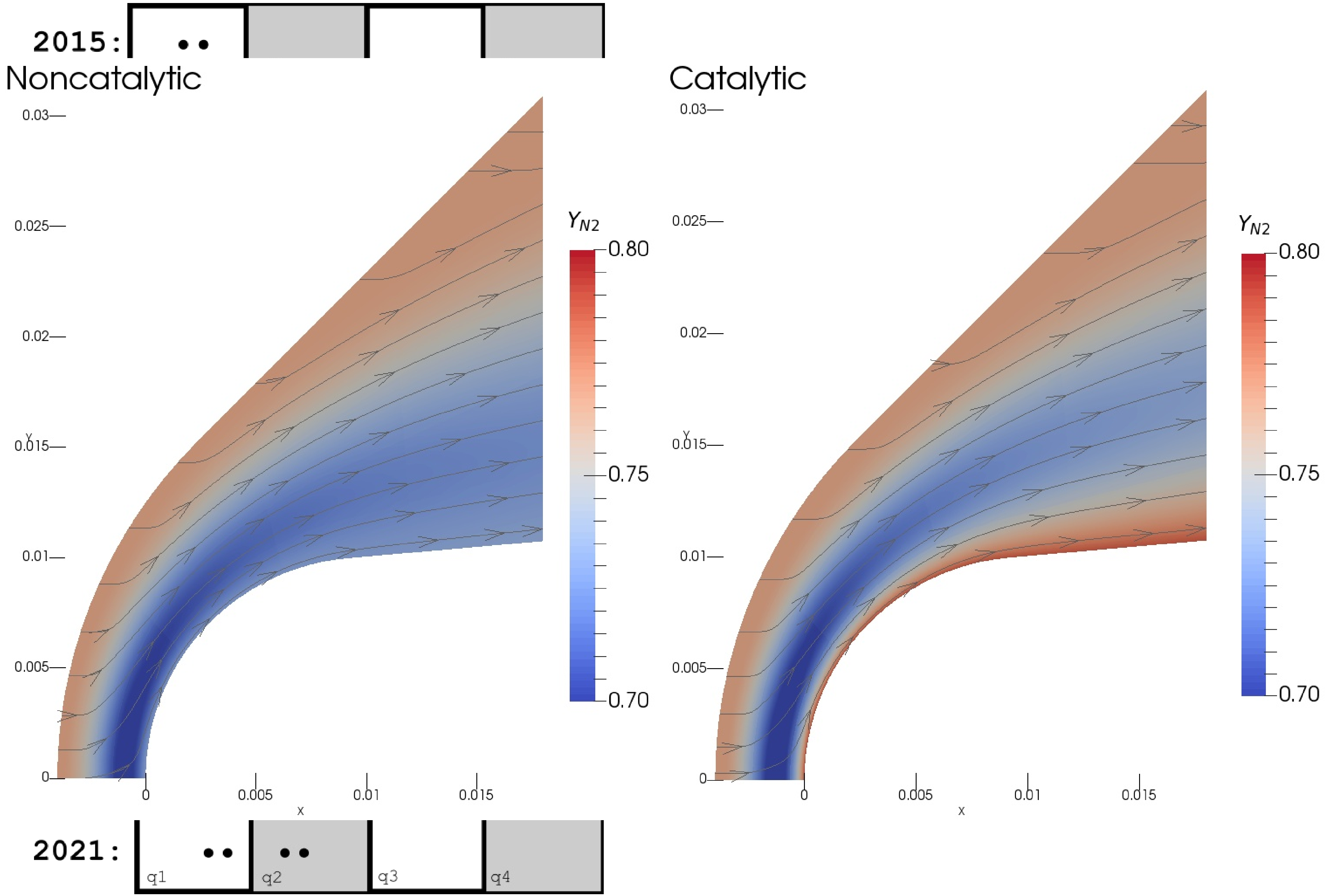


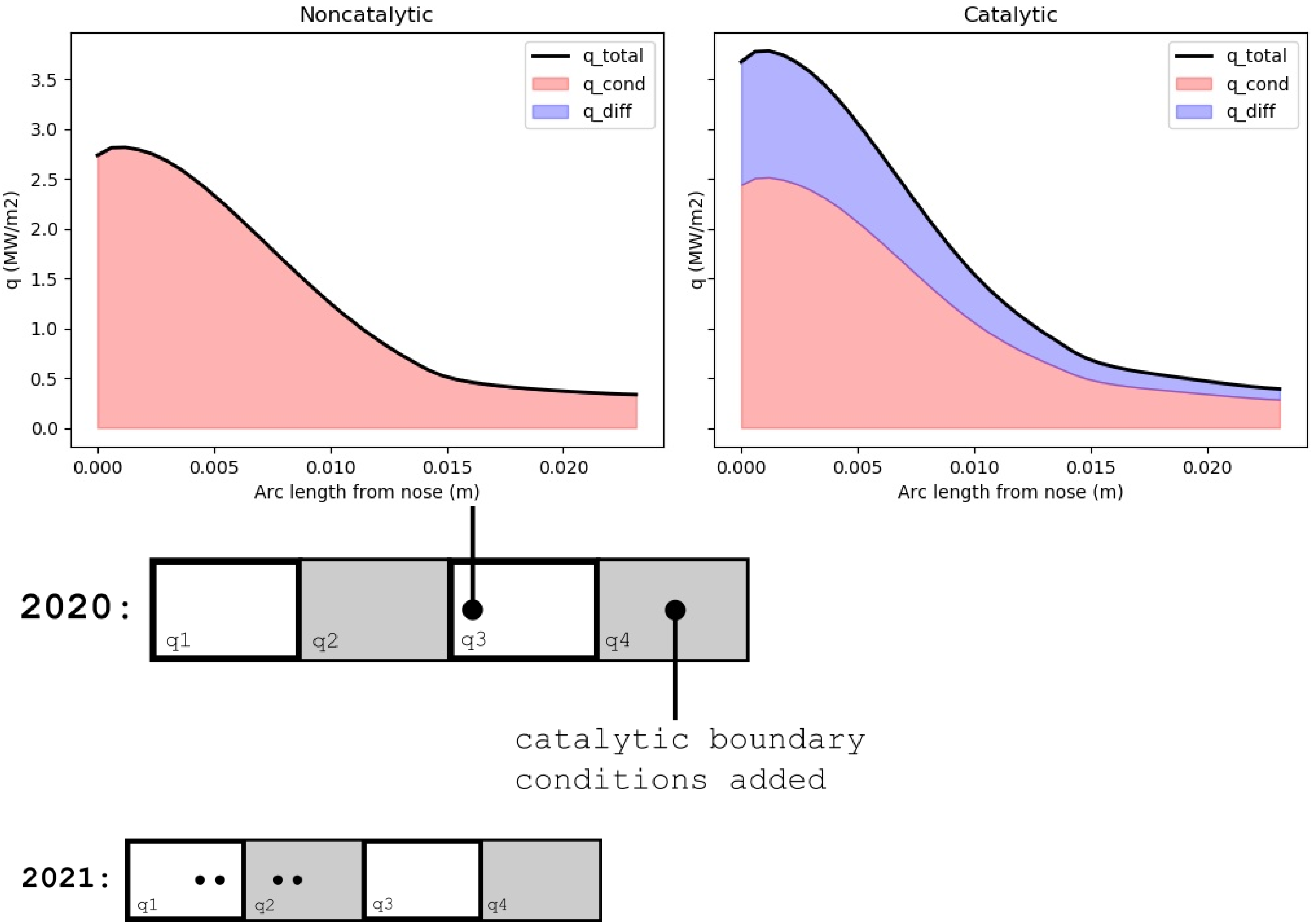
2015:
q1
q2
q3
q4
2017:
q1
chemki
2018:
2-T ai
(Gnoff
2019:
q1
2020:
q1
2021:
q1
q2
q3
q4
Shock shape in front of a sphere fired in air
R_n = 7.0mm, u_∞ = 3.49 km/s, p_∞ = 4850 Pa, $\rho_\infty R_n$ = 4.0e-4 kg/m^2
experiment, upper side
experiment, lower side
eilmer, 2-T air model
Δ/R_n
θ, degrees
0
0.1
0.2
0.3
0.4
0.5
0.6
10
20
30
40
50
60
70
80
90

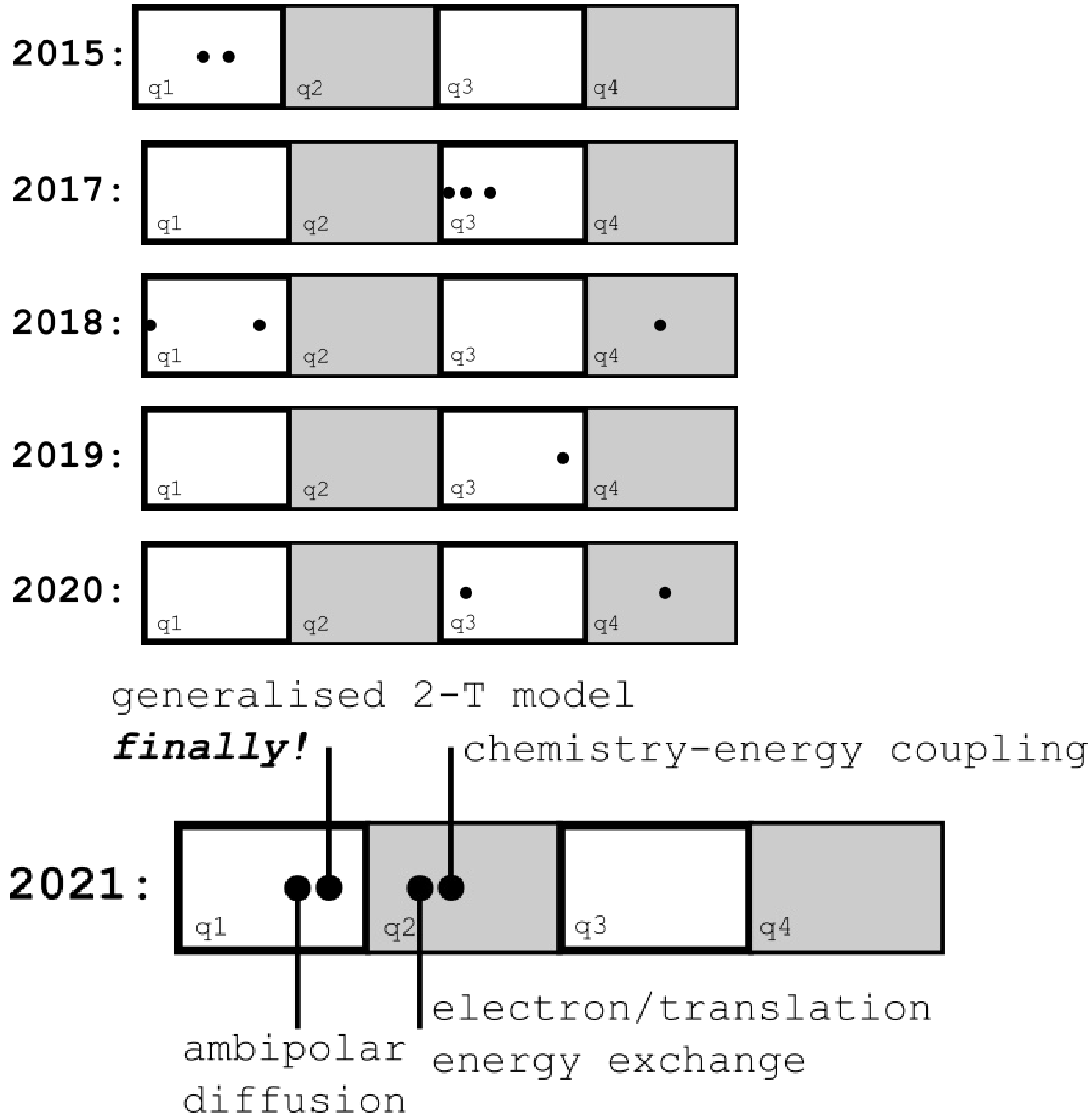


2015:
q1
q2
q3
q4
2017:
q1
q2
q3
q4
2018:
q1
q2
q3
q4
2-T dissociating nitrogen model
2019:
q1
q2
q3
q4
2020:
q1
q2
q3
q4
2021:
q1
q2
q3
q4

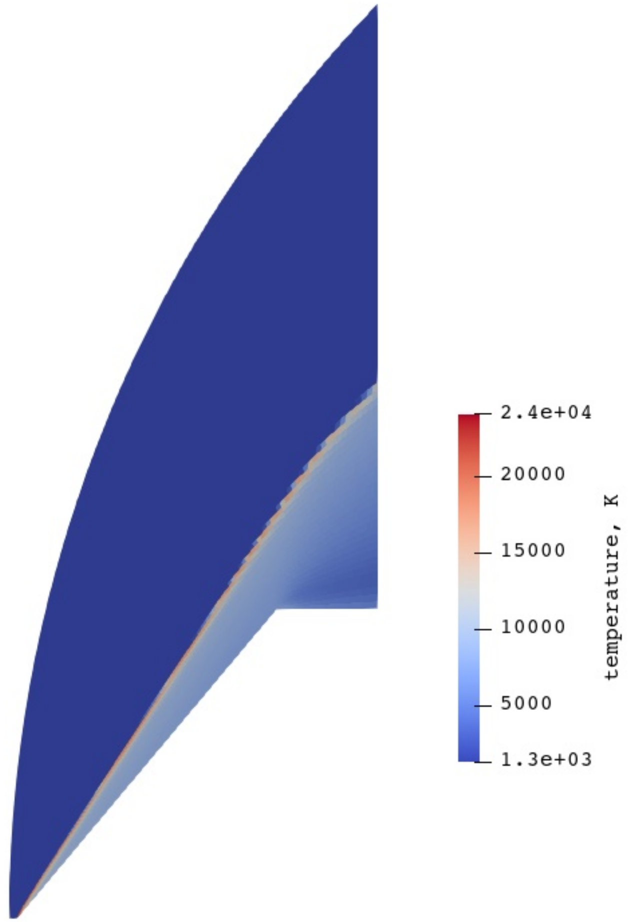

2015:
q1
q2
q3
q4
2017:
2018:
2019:
curve fits to 50,000 K
for N, O, N+, O+
2020:
catalytic boundary
conditions added
2021:


2015:
Noncatalytic
Catalytic
Y_{N2}
0.80
0.75
0.70
0.03
0.025
0.02
0.015
0.01
0.005
0
y
x
2021:
q1
q2
q3
q4

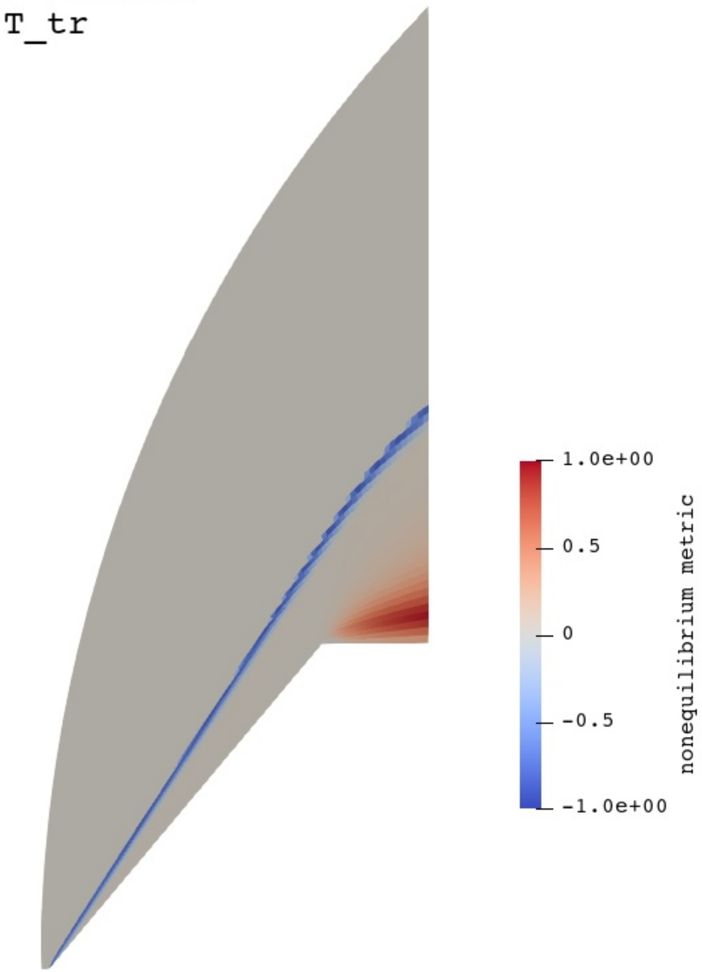

Noncatalytic
Catalytic
q_total
q_cond
q_diff
q (MW/m2)
Arc length from nose (m)
0.000
0.005
0.010
0.015
0.020
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
2020:
q1
q2
q3
q4
catalytic boundary
conditions added
2021:
q1
q2
q3
q4


2015:
q1
q2
q3
q4
2017:
q1
q2
q3
q4
2018:
q1
q2
q3
q4
2019:
q1
q2
q3
q4
2020:
q1
q2
q3
q4
generalised 2-T model
finally!
chemistry-energy coupling
2021:
q1
q2
q3
q4
electron/translation
energy exchange
ambipolar
diffusion

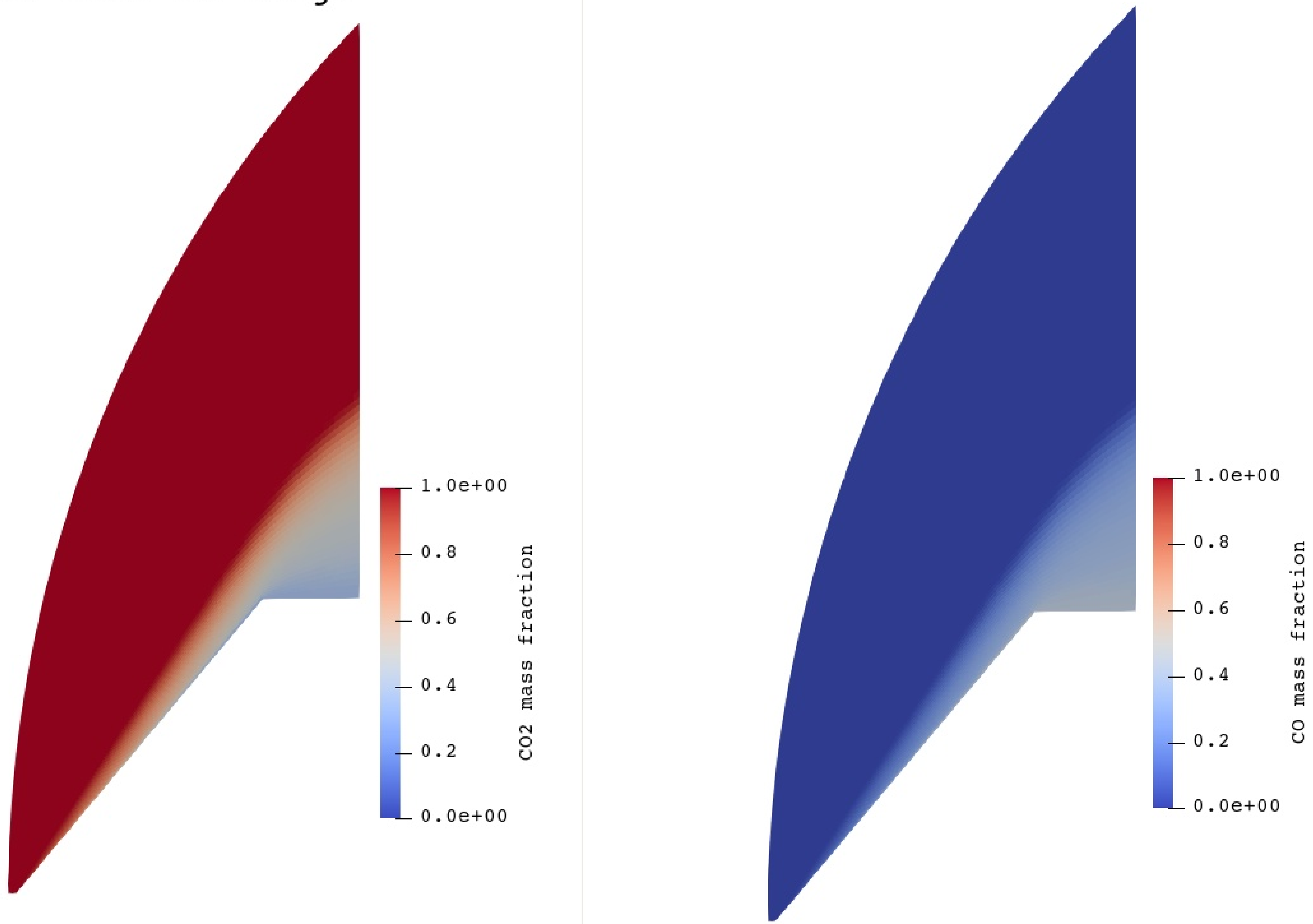
CO2 flow over 2D wedge



nonequilibrium metric:
(T_v - T_tr)/T_tr



CO2 flow over 2D wedge



III: Steady-state accelerator development

2016

[OCT] RJG (7cc267..) : implemented 2D single-block version of Newton-Krylov solver on structured grids, tested on an inviscid Mach 10 flow over a 6 degree wedge.

[NOV] RJG (a27b9e..) : added restarted flexible GMRES and GMRES iterative preconditioner, tested on a Mach 4 laminar flat plate test case
[NOV] RJG (0c8bda..) : extended solver to operate on unstructured grids
[NOV] RJG (401978..) : shared-memory parallel version

2017

[MAR] RJG (b57c0c..) : extended solver to 3D flows
[JUN] RJG (9c28d6..) : extended solver to RANS equations (k-omega turbulence model)

III: Steady-state accelerator development

2018

[JUN] KAD (9f1581..) : solver now operates using complex-numbers (complex Frechet derivative variant and complex-step preconditioner)
[JUL] KAD (304ef9..) : block-Jacobi preconditioner now operates using complex-step differentiation
solver exhibits textbook convergence for the inviscid supersonic ramp test case in the paper by Marques and Pereira
[JUL] KAD (7ee999..) : added ILU(0) preconditioner and lagged preconditioner option
[SEP] KAD (c58f79..) : re-implemented equation and variable scaling based on Brown and Hindmarsh (1986) paper, improved scaled simulations which were performing poorly
[NOV] KAD (f981f8..) : extend precondition matrix construction to 3D

2020

[APR] RJG (cfc1bd..) : MPI extension
[JUN] KAD (75b697..) : local time-stepping now compatible with Newton-Krylov solver
[JUN] KAD (eb6b59..) : user-defined CFL schedule
[SEP] KAD (aa1430..) : experimented with matrix-free LU-SGS method as a preconditioner
[OCT] KAD (347164..) : extended solver to reacting (finite-rate chemistry) multispecies flows

III: Steady-state accelerator development

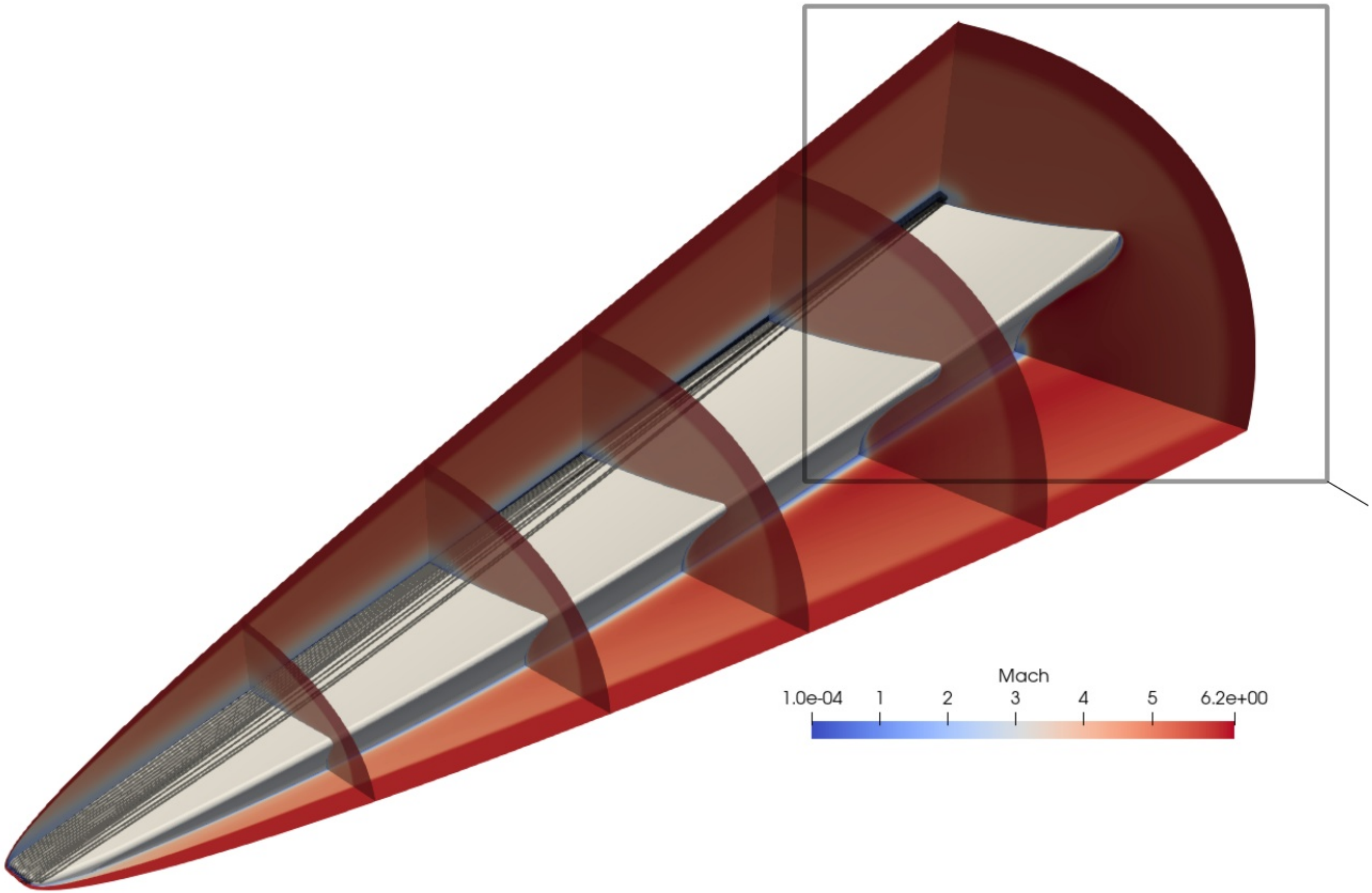
2021

[APR] KAD (1347d9..) : extended Newton-Krylov solver to operate on solid domains
[MAY] KAD (51ed07..) : added multi-temperature capability
[JUN] KAD (fcb560..) : spatial order of accuracy of LHS and RHS can be set independently
[JUL] KAD (cc0c33..) : added block Symmetric Gauss-Seidel (SGS) preconditioner
[AUG] KAD (652e80..) : re-implemented real-valued version using perturbation equation from Knoll's papers
[SEP] KAD (082d91..) : added relaxation factor via a physicality check

----
2022

[FEB] KAD (41140d..) : refactor of Newton-Krylov algorithm to be driven by the physicality check - solver is much more robust now
[MAR] KAD (03b9aa..) : finally removed the mass continuity equation for multispecies flows, reacting simulations are much more stable now!
[MAR] KAD (cb9ff2..) : added in reverse Cuthill-McKee cell reordering
[MAR] KAD (e6514f..) : added in ILU(k) preconditioner

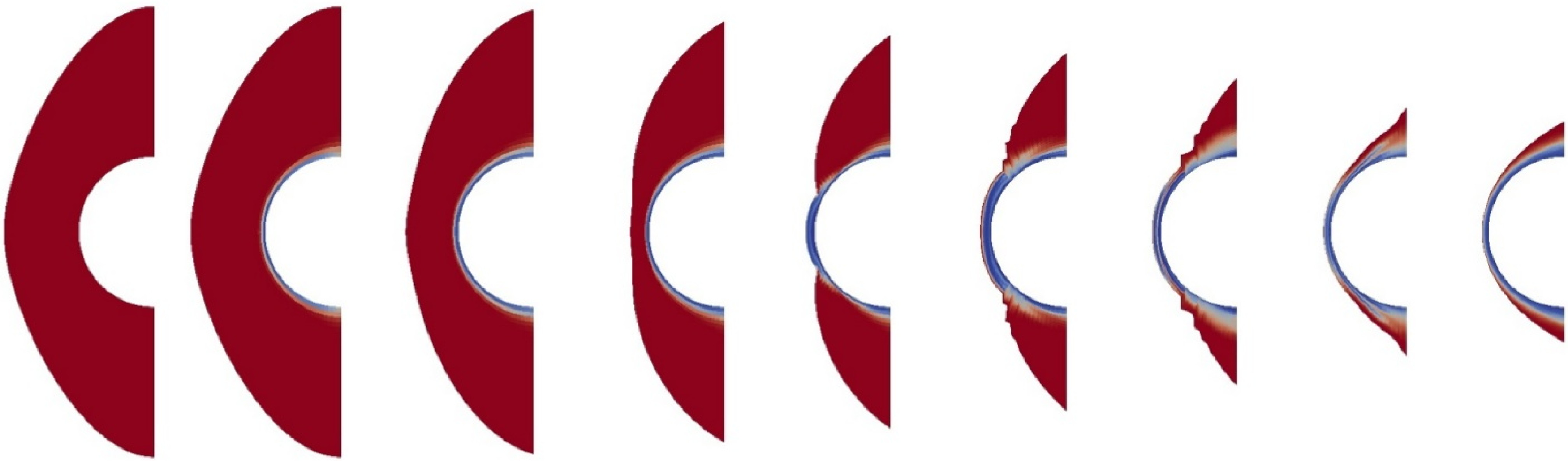
III: Steady-state accelerator development



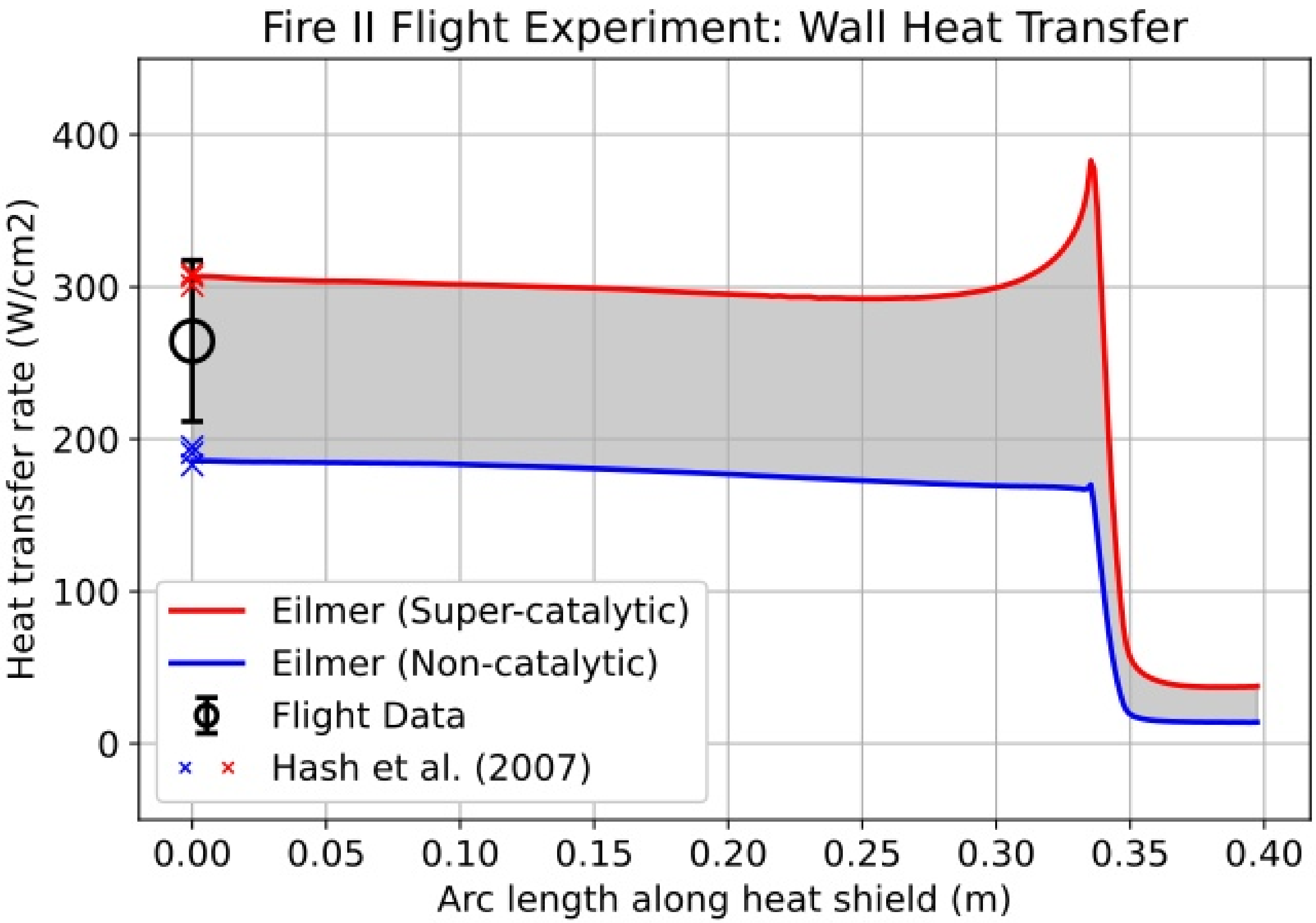
IV: Concluding remarks

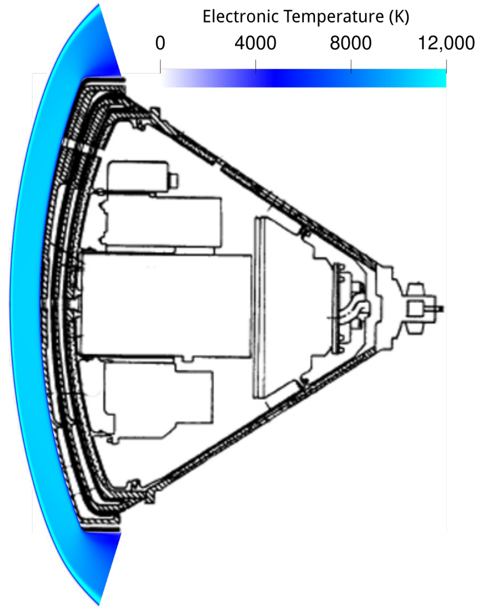
Recommended simulation process for estimating heat transfer

1. coarse inviscid shock-fitting simulation
2. extract grid, tailor and cluster
3. coarse viscous simulation
4. perform grid refinements



IV: Concluding remarks: does it work?





IV: Concluding remarks

Estimating convective heating for FireII

+ shock-fitting
+ high-quality grid generation
+ accelerator for steady-state
+ nonequilibrium (multi-temperature) thermodynamics
+ nonequilibrium transport properties
+ wall-catalytic boundary conditions
+ finite-rate chemistry (w multi-T effects)
+ energy exchange mechanisms

What's left to do (in the short term) ...

+ generalised 3-T model (Rob Watt)
+ state-specific CO-X model (Nick Gibbons)
+ loosely-coupled CHT simulations (Kyle Damm)
+ coupling to radiation
+ ......