Adaptive Nuclear Statistical Equilibrium for Type Ia SN Simulation

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INTRODUCTION

Due to the stiff nature of solving reaction equations for simulating thermonuclear explosions, i.e. Type Ia SN and X-ray bursts, these simulations require careful coupling of hydrodynamics and reactions to avoid being limited by the nuclear reaction timescale instead of hydrodynamic timescale. But as temperature reaches beyond ~ 6 billion Kelvin, numerical integration becomes even more challenging when the timescale of the composition to reach statistical equilibrium is much shorter than the sound crossing time. Inspired by earlier work [1, 2] in the community at adaptively evaluating the nuclear statistical equilibrium (NSE) conditions, we have implemented an adaptive NSE method in our simplified spectral-deferred-corrections (SDC) [3] coupling of hydrodynamics and reactions. This can seamlessly transition from integrating a network to imposing the equilibrium during the reaction update of a simulation.

In this work, we demonstrate the recent effort of implementing an adaptive NSE algorithm in Castro/Microphysics code. We will show case its viability using a 2D sub-chandrasekhar double-detonation progenitor model for type Ia SN.

NUCLEAR STATISTICAL EQUILIBRIUM

Nuclear Statistical Equilibrium: An equilibrium state of the system where the forward and reverse strong reactions are in chemical equilibrium. By imposing chemical equilibrium, one can derive the equation, Eq. 1, of determining the composition in NSE subject to two constraints, conservation of mass (Eq. 2) and charge (Eq. 3) given (T, ρ, Y_e). So, we can do an algebraic solve (we use Hybrid-Powell Method) to avoid the expensive integration!

$$X_i = \frac{m_i}{\rho} g_i \left(\frac{2\pi m_i k_B T}{h^2}\right)^{3/2} \exp\left(\frac{Z_i \mu_p + N_i \mu_n + Q_i - \mu_i^C}{k_B T}\right)$$

Eq. 1: NSE Composition Equation with two unknowns: μ_p and μ_n

$$\Sigma_i X_i = 1$$

Eq. 2: Conservation of baryon #

$$Y_e = \Sigma_i \frac{Z_i}{A_i} X_i$$

Eq. 3 : Conservation of charge.

REFERENCES

[1] Kushnir, D., & Katz, B. (2020). DOI: 10.1093/mnras/staa594

[2] Lippuner, J., & Roberts, L. (2018). DOI: 10.3847/1538-4365/aa94cb

[3] Zingale, M., Katz, M. P., Nonaka, A., & Rasmussen, M. (2022). DOI: 10.3847/1538-4357/ac8478

[4] Zingale, M., Chen, Z., Rasmussen, M., Polin, A., Katz, M. P., Clark, A., S., & Johnson, E. (2024). DOI: 10.3847/1538-4357/ad3441

CODE

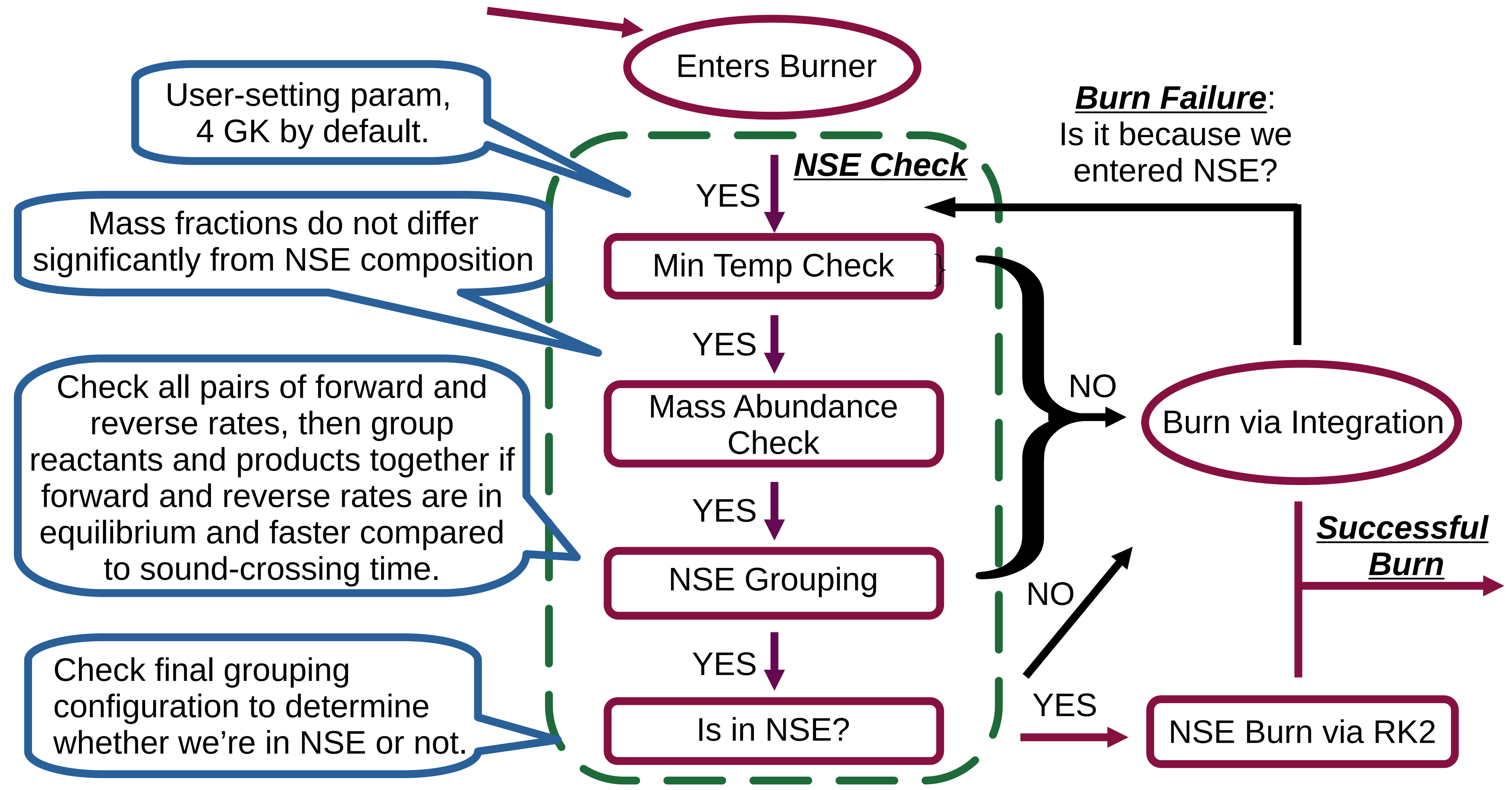
Castro | https://github.com/AMReX-Astro/Castro

Microphysics | https://github.com/AMReX-Astro/Microphysics

Pynucastro | https://github.com/pynucastro/pynucastro

New Contributions Are Welcome!

NSE EVOLUTION SCHEMATIC DIAGRAM



CONVERGENCE

Field	$\epsilon_{32\to64}$	rate	$\epsilon_{64\to128}$	rate	$\epsilon_{128\to256}$	rate	$\epsilon_{256\to512}$
ρ	3.58e+19	1.948	9.27e+18	2.033	2.27e+18	2.042	5.50e+17
ρu	1.80e+28	1.036	4.37e+27	2.002	1.09e+27	1.988	2.75e+26
ρv	1.80e+28	2.046	4.37e+27	2.002	1.09e+27	1.988	2.75e+26
ρE	5.41e+37	1.955	1.39e+37	2.021	3.44e+36	1.999	8.60e+35
ρe	5.33e+37	1.955	1.38e+37	2.022	3.39e+36	1.999	8.50e+35
T	5.86e+20	2.000	1.46e+20	2.131	3.34e+19	2.278	6.90e+18
$\rho X(^4\mathrm{He})$	2.83e+18	1.859	7.79e+17	2.014	1.93e+17	2.227	4.12e+16
$\rho X(^{48}\mathrm{Cr})$	1.22e+18	2.041	2.98e+17	2.214	6.41e+16	2.242	1.36e+16
$\rho X(^{52}\mathrm{Fe})$	1.43e+19	1.903	3.82e+18	1.999	9.55e+17	2.076	2.27e+17
$\rho X(^{56}\mathrm{Ni})$	3.88e+20	2.038	9.44e+19	2.086	2.22e+19	2.228	4.74e+18

Table 1: This shows the convergence rates using the L_1 Norm for NSE convergence test problem along with simplified-SDC coupling. This shows that NSE burn is 2nd order accurate.

TEST PROBLEM

Background: We use run 2-D Type Ia SN simulations of a sub-Chandrasekhar mass white dwarf with an accreted He layer and a C/O core [4]. This is a double detonation model where the detonation wave caused by He burning sends out a compression wave that eventually propagates inward and ignites the core causing a second C detonation. During the second detonation, integrating the network becomes extremely difficult as T reaches beyond 6 GK, suggesting NSE taken place. To test the NSE evolution mode, is to make sure we get approximately the same solution with NSE evolution disabled, and faster at the same time.

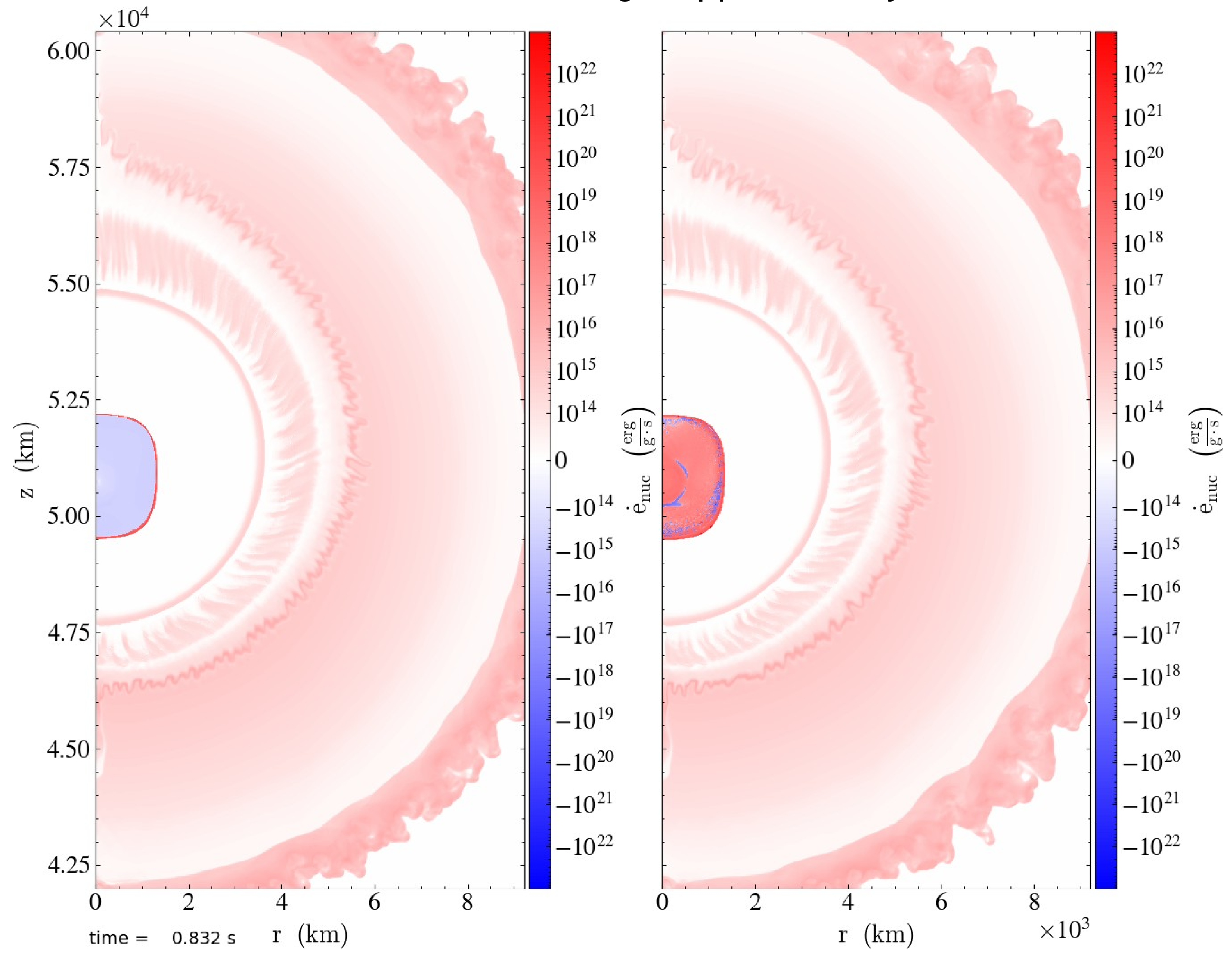


Fig 1: Slice plots showing the specific nuclear energy generation rate for the sub-Chandrasekhar Type-Ia SN model. ***Left:*** NSE evolution enabled. ***Right:*** With NSE evolution disabled. We successfully detects NSE within the second detonation. The energy update is not fully correct, due to missing terms in the energy update, which ended up suppressing the energy output. This issue has been fixed recently.

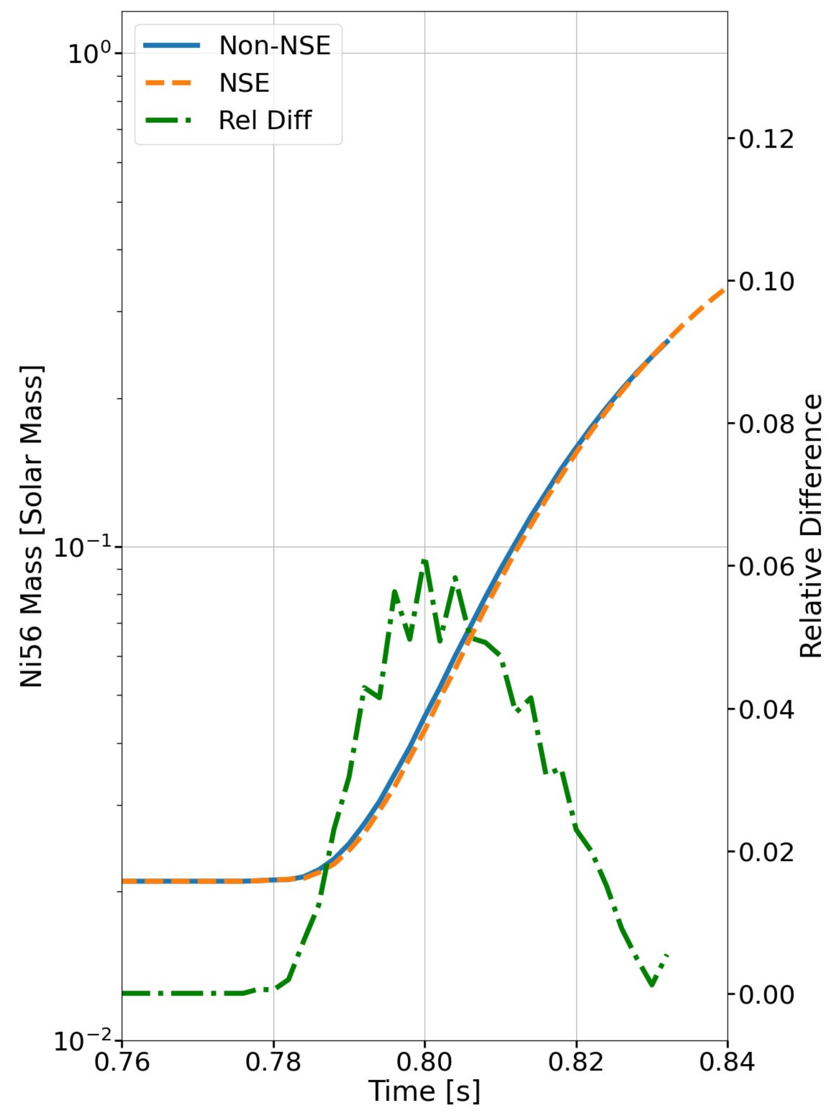


Fig 2: Ni56 Mass evolution plot in solar mass unit. Axis on the right shows the relative difference. At ~0.78 s, C detonation happens and we see a sharp increase in Ni56. We see that NSE evolution mode agrees well with NSE disabled.

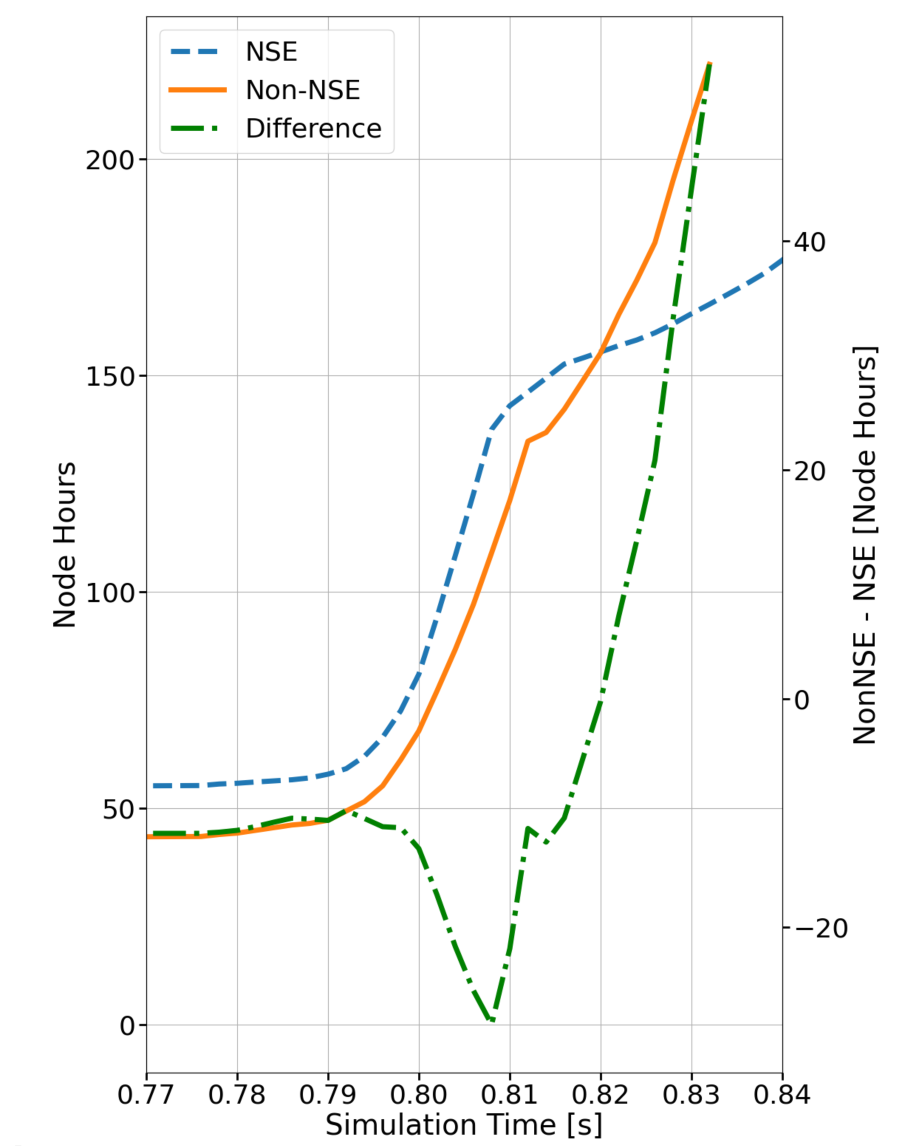


Fig 3: Node hours taken to run simulations. Before C detonation, NSE run is slower due to the NSE detection algorithm overhead. After C detonation, NSE run is slower initially, but ended up being faster after using the Jacobian-swap trick. Jacobian-swap refers to switching between numerical and analytic Jacobian during a burning-retry after integration fails. While one type of Jacobian struggles with integration, we find the other type usually solves the system instantly.

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