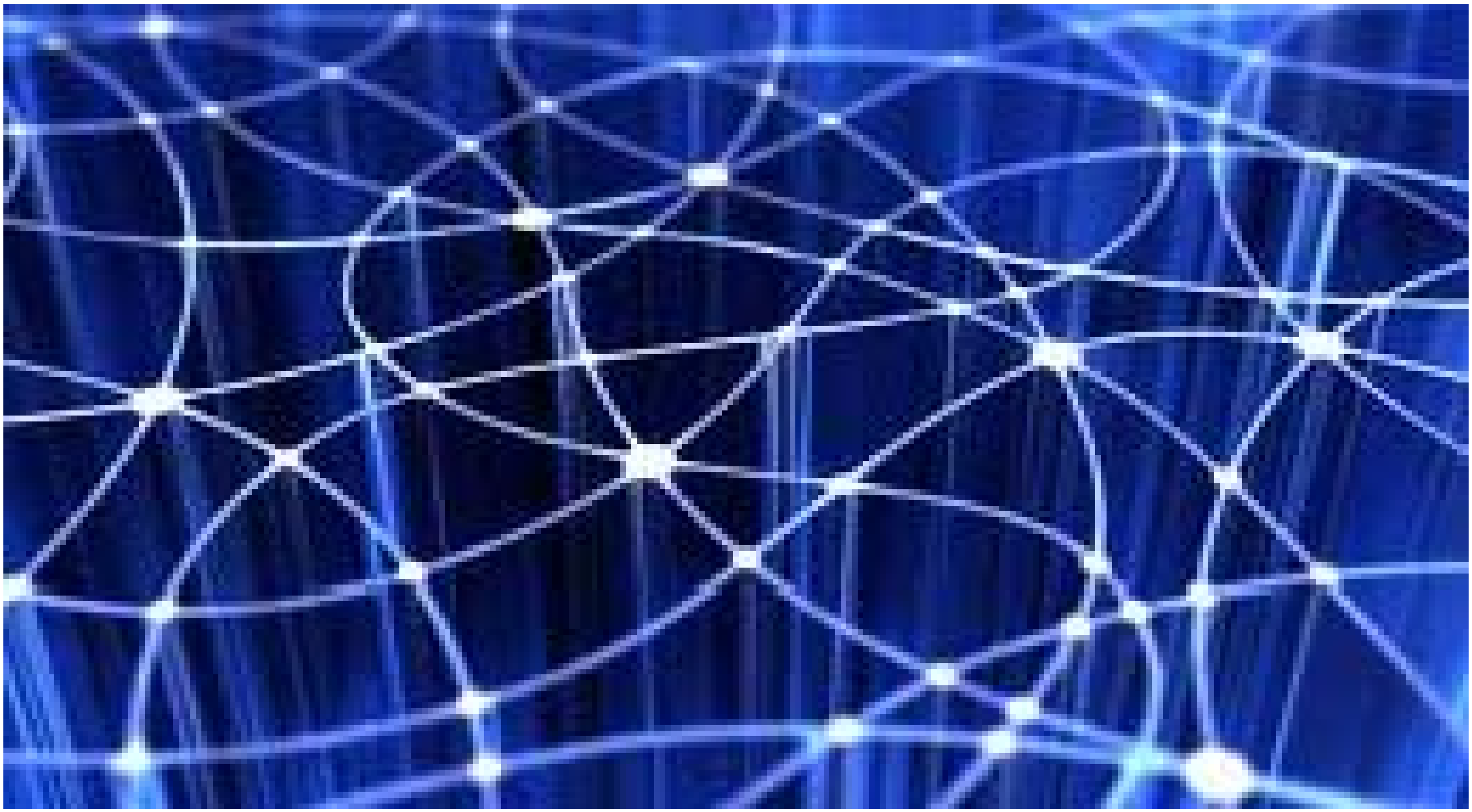
Solving Reaction Networks



General reaction network

A set of n isotopes with abundances Y_i,

Consider 1- and 2-body rates only, these rates can produce or destroy each isotope

$$\frac{dY_i}{dt} = \underbrace{\left[\sum_{j,k} Y_j Y_k \rho N_A < \sigma v >_{jk \to i} + \sum_l \lambda_{l \to i} Y_l \right]}_{\text{production}}$$

$$- \underbrace{\left[\sum_m Y_i Y_m \rho N_A < \sigma v >_{im \to \text{any}} + \sum_n \lambda_{i \to n} Y_i \right]}_{\text{destruction}}$$

production

destruction

Note that this depends on mass density ρ and temperature (through $<\sigma v>$ and λ) so this requires input from a stellar model.

Needs to be solved numerically. This is not trivial as system is very stiff (reaction rate timescales vary by many many orders of magnitude)

Solving reaction networks numerically

General problem:

Vector of abundances at time t $Y_i(t)$

Set of differential equations (the reaction network) $\frac{dY_i}{dt} = f(\vec{Y})$

Want to calculate $Y_i(t+\Delta t)$ from $Y_i(t)$ so need $\Delta Y_i = Y_i(t+\Delta t) - Y_i(t)$

Simplest explicit approach:

$$\Delta Y_i = f(\vec{Y}(t))\,\Delta t$$

Problem: as system is very stiff (rates vary by many orders of magnitude) this requires extremely small time steps, and so at least in its simplest form this is not practical

Solving reaction networks numerically

Simplest implicit approach:

$$\Delta Y_i = f(\vec{Y}(t+\Delta t))\,\Delta t \quad (1)$$

To first order:

$$f_i(\vec{Y}(t+\Delta t)) = f_i(\vec{Y}(t)) + \sum_j \boxed{\frac{\partial f_i(\vec{Y}(t))}{Y_j}}\,\Delta Y_j + \ldots$$

Jacobian J_{ij}

Insert into (1):

$$\frac{\Delta Y_i}{\Delta t} = f_i(\vec{Y}(t)) + \sum_j J_{ij}\Delta Y_j$$

Solving reaction networks numerically

Or in vector/matrix notation:

$$\frac{\Delta\vec{Y}}{\Delta t} = \vec{f}(t) + \tilde{J}\Delta\vec{Y}$$

Solve for ΔY:

$$\frac{\Delta\vec{Y}}{\Delta t} - \tilde{J}\Delta\vec{Y} = \vec{f}(t) \quad \rightarrow \quad \Delta\vec{Y}\left(\frac{\tilde{1}}{\Delta t} - \tilde{J}\right) = \vec{f}(t)$$

$$\rightarrow \quad \Delta\vec{Y} = \vec{f}(t)\left(\frac{\tilde{1}}{\Delta t} - \tilde{J}\right)^{-1}$$

Main numerical task:
Setup this matrix and invert it