^{163}Lu - New Formalism for the TSD4 Band

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Detailed report with regards to the implementation of a C++ algorithm for finding the best parameter set which reproduces the wobbling spectrum of ^{163}Lu.

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1 Mathematical problem

We address the initial-value problem

$$u'(t) = -au(t), \quad t \in (0, T], \tag{1}$$
$$u(0) = I, \tag{2}$$

where a, I, and T are prescribed parameters, and $u(t)$ is the unknown function to be estimated. This mathematical model is relevant for physical phenomena featuring exponential decay in time, e.g., vertical pressure variation in the atmosphere, cooling of an object, and radioactive decay.

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2 Numerical solution method

We introduce a mesh in time with points $0 = t_0 < t_1 \cdots < t_{N_t} = T$. For simplicity, we assume constant spacing Δt between the mesh points: $\Delta t = t_n - t_{n-1}$, $n = 1, \ldots, N_t$. Let u^n be the numerical approximation to the exact solution at t_n.

$$u^{n+1} = \frac{1 - (1-\theta) a \Delta t}{1 + \theta a \Delta t} u^n,$$

for $n = 0, 1, \ldots, N_t - 1$. This scheme corresponds to

- The Forward Euler scheme when $\theta = 0$
- The Backward Euler scheme when $\theta = 1$
- The Crank-Nicolson scheme when $\theta = 1/2$

3 Implementation

```
def solver(I, a, T, dt, theta):
    """Solve u'=-a*u, u(0)=I, for t in (0,T] with steps of dt."""
    dt = float(dt)              # avoid integer division
    Nt = int(round(T/dt))       # no of time intervals
    T = Nt*dt                   # adjust T to fit time step dt
    u = zeros(Nt+1)             # array of u[n] values
    t = linspace(0, T, Nt+1)    # time mesh

    u[0] = I                    # assign initial condition
    for n in range(0, Nt):      # n=0,1,...,Nt-1
        u[n+1] = (1 - (1-theta)*a*dt)/(1 + theta*dt*a)*u[n]
    return u, t
```

4 Numerical experiments

Δt	$\theta = 0$	$\theta = 0.5$	$\theta = 1$
1.25	7.4630	0.2161	0.2440
0.75	0.6632	0.0744	0.1875
0.50	0.2797	0.0315	0.1397
0.10	0.0377	0.0012	0.0335

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