



LSODA Stiff Solver

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LSODA.cpp

LSODA stands for *Livermore Solver for Ordinary Differential equations with Automatic method switching* written by Alan C. Hindmarsh and Linda R. Petzold.

Paper – https://computing.llnl.gov/sites/default/files/ODEPACK_pub1_u88007.pdf

LSODA Features

Hybrid Solver – Combines two methods: fast Adams predictor–corrector for nonstiff regions and stable implicit Backwards Differentiation (BDF) for stiff regions, switching automatically when stiffness is detected.

Stiffness Detection – Monitors error growth vs. step size; switches to BDF before instability occurs, so it never wastes time taking thousands of tiny steps like ode.cpp.

Adaptive Step Size & Order – Continuously tunes both step length and polynomial order for efficiency and accuracy, ensuring minimal computation while meeting tolerance requirements.

Banded Jacobian Support – Can exploit narrow bandwidth in ETACHA's Jacobian, cutting stiff-solve cost and giving massive speed-ups for large systems.



Implementation

Why LSODA Needs Banded Jacobians

- Banded LU slashes cost and memory(~60%).
- Potentially **1000× faster** in stiff phases.

Why LSODA is Faster When Stiff

- Detects stiffness early, switches to large stable implicit steps.
- ode.cpp shrinks steps until max-step error; LSODA leaps over stiff bottleneck.

LSODA Advantages

- **Euler, Adams PECE, RK45** all work well for non-stiff problems but fail or become extremely slow when stiffness appears.
- **LSODA** automatically switches between non-stiff (Adams) and stiff (BDF) methods, so it can handle both without user intervention.

LSODA.cpp is around 60% faster than the original Fortran version EQDIF.for.



LISE package

ETACHA4 - eUntitled

File Execute Help

Projectile

A	Element	Z	Q
207	Pb	82	64

Last orbital of

Neutral atom = 6 p 2

Ion in ground state = 3 p 6

Energy (MeV/u)

	Initial	Final	
28.9	75.905	28.532	76.335

Stopping power (MeV/mg/cm²)

Use Energy Loss Calculations

Target

A	Element	Z
12	C	6

Thickness = 5.018e+19 atoms/cm²

Density = 2.26 g/cm³

Reaction characteristics

perturbation parameter Kp (n=1) = 0.18

Kp (n=3) = 0.02

projectile velocity V_z = 33.364 au

Version

☐ v.23 Y(1s,2s,2p),Y(3s),Y(3p),Y(3d)

☒ v.3 + Y(12,3) fast, for high E

☐ v.34 + Y(4) do not use

☐ v.4 + Y(123, 4) recommended

☐ v.45 + Y(5) beta

IONIZATION model

☒ CDW-EIS (default)

☐ PWBA (fast)

EXCITATION model

☒ Symmetric-Eikonal (default)

☐ PWBA (fast)

Integration model

☐ ODE ISBN: 0716704617 (ordinary differential equation solver)

☐ RK45 (Runge-Kutta-Fehlberg ODE solver)

☐ Euler's method

☒ LSODA (Stiff Solver)

Steps & Numerical uncertainties

Absolute = 1.00e-8

Relative = 1.00e-4

Minimum step = 5 μg/cm²

Maximum step = 2000 μg/cm²

Show Results

Event Logs

☐ Intermediate output of cross sections

☒ Plots (General set)

☒ Charge state evolution plot

☐ Debug mode

Finished at 00:55:23

Elapsed time is 00:00:01 (or 1.795 sec)

Final energy: 28.458 (MeV/u)

output data in files:

00 to 06 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta0000.txt

10 to 16 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta1010.txt

20 to 26 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta2020.txt

30 to 36 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta3030.txt

40 to 46 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta4040.txt

50 to 56 EE- charge states in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_Eta5050.txt

base 1s,2s,2p, 1s2, 1s2s, 1s2p, 1s2 2s, 1s2+2p ions and sum of these in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_ETAPIED.txt

mean 1s,2s,2p,3s,3p and 3d populations in /Intranet.nsl.msu.edu/files/user/tarasov/My Documents/LISEout/results/eUntitled_POPMEAN.txt

WARNING! Next calculation will overwrite these files. Consider saving or renaming these results!

FINAL achieved >> T=1.000 mg/cm² <Q>=73.267 dQ=1.166 E=28.458 dSum=2.000

Ready