

Forward Solver D-Stability Study

Automated Benchmark Report

February 11, 2026

What We Ran

Goal

This study maps where the forward PNP solve converges or fails as (D_0, D_1) varies.

Setup

Study mode: Anisotropy-dense grid. Grid points: 1465. Coarse global grid with dense sampling concentrated where $\max(D_0, D_1)/\min(D_0, D_1) \approx 8$. Composition: `global.coarse=324, lbfgsb_focus=196, anis_lowD0_highD1=380, anis_highD0_lowD1=67, anis_extreme_lowD0_highD1=287, anis_extreme_highD0_lowD1=100`. Non- D parameters match the inverse studies: $n_{\text{species}} = 2$, $dt = 0.02$, $t_{\text{end}} = 0.1$, $z = [1, -1]$, $a = [0, 0]$, $c_0 = [0.1, 0.1]$, $\phi_0 = 1.0$, SNES newtonls + LU/MUMPS.

How to read the map

Colored cells are converged solves with color = wall time (seconds, lower is better); red x marks failed solves. The dashed diagonal marks $D_0 = D_1$.

Summary Metrics

Metric	Value
Total (D_0, D_1) points	1465
Converged points	830
Failed points	635
Success rate	56.655%
Median converged solve time (s)	1.0117
Failure reasons	DIVERGED_LINE_SEARCH: 428, DIVERGED_MAX_IT: 207

D-Stability Map

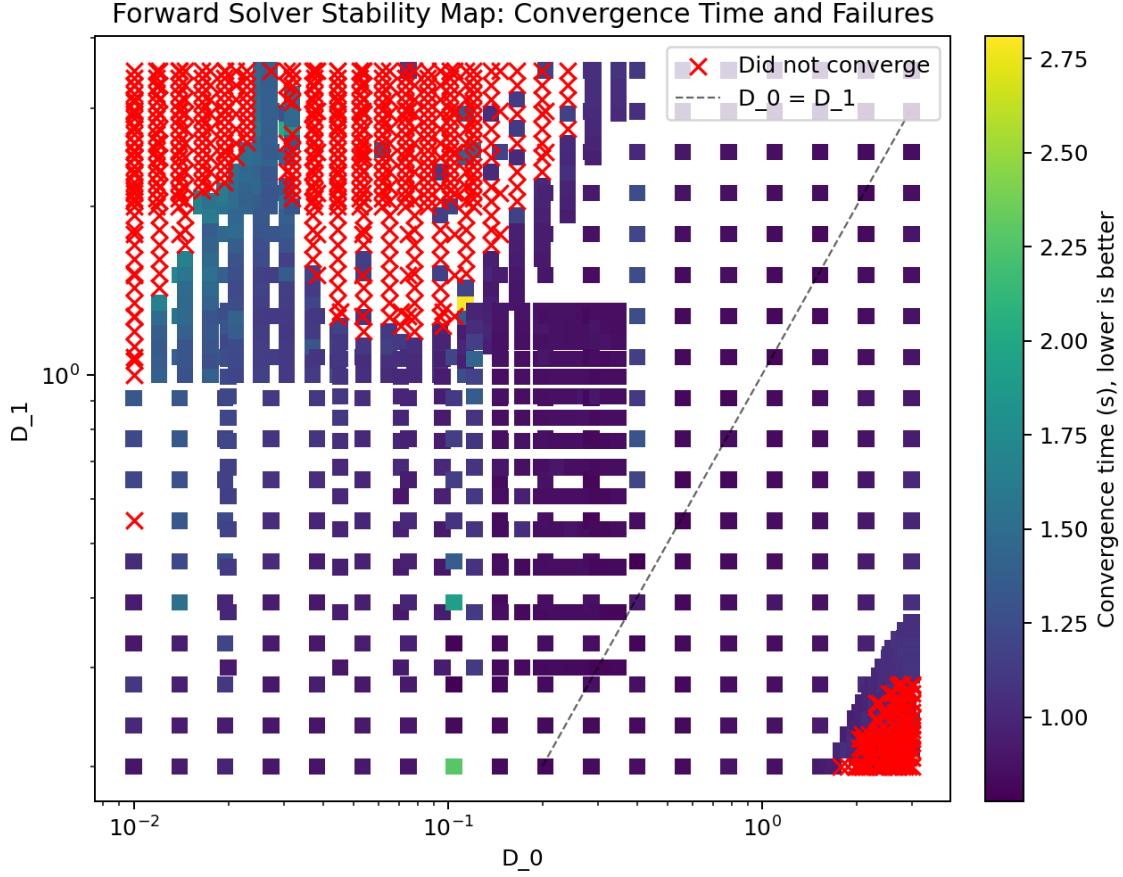


Figure 1: Forward-solver behavior in (D_0, D_1) space. Dashed line marks $D_0 = D_1$. Converged time is lower-is-better.

Failure Pattern Summary

Failures span $D_0 \in [0.01, 3]$ and $D_1 \in [0.2, 3.5]$, but cluster most strongly in low-and-imbalanced diffusion regimes. Median $\min(D_0, D_1)$ is 0.06186 for failed points vs 0.2 for converged points; median anisotropy max / min is 39.46 vs 8.813.

Region	Failures / Points	Failure Rate (%)
LBFGS-B focus: $D_0 \in [0.02, 0.35], D_1 \in [0.3, 1.3]$	14 / 321	4.361
High anisotropy: $\max(D_0, D_1) / \min(D_0, D_1) \geq 10$	612 / 948	64.56
Extreme corner: $\min(D) \leq 0.1, \max(D) \geq 2.5$	216 / 244	88.52
Low- D_0 /high- D_1 : $D_0 \leq 0.1, D_1 \geq 1.3$	408 / 517	78.92
High- D_0 /low- D_1 : $D_0 \geq 1.0, D_1 \leq 0.35$	119 / 293	40.61

Representative Failed Points

D_0	D_1	Time (s)	Failure reason
0.01	0.5492	0.9255	DIVERGED_LINE_SEARCH
0.01	1	0.9592	DIVERGED_LINE_SEARCH
0.01	1.061	1.005	DIVERGED_LINE_SEARCH
0.01	1.077	1.514	DIVERGED_MAX_IT
0.01	1.127	0.9722	DIVERGED_LINE_SEARCH
0.01	1.196	1.039	DIVERGED_LINE_SEARCH
0.01	1.269	1.307	DIVERGED_MAX_IT
0.01	1.275	0.9961	DIVERGED_LINE_SEARCH
0.01	1.348	1.107	DIVERGED_LINE_SEARCH
0.01	1.43	1.293	DIVERGED_LINE_SEARCH

Full failed-point list is available in `forward_solver_d_stability_results.csv`.

Interpretation

- The dominant failure mode is DIVERGED_LINE_SEARCH, indicating globalization difficulty in SNES Newton steps.
- Failure probability rises sharply when one diffusion coefficient is small and the other is large (strong imbalance).
- This explains the inverse-study behavior: methods that step through highly imbalanced D trial points are more likely to trigger forward-solve failures.