

Example Programs for CVODES

v7.1.1

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CONTRIBUTORS

The SUNDIALS library has been developed over many years by a number of contributors. The current SUNDIALS team consists of Cody J. Balos, David J. Gardner, Alan C. Hindmarsh, Daniel R. Reynolds, and Carol S. Woodward. We thank Radu Serban for significant and critical past contributions.

Other contributors to SUNDIALS include: James Almgren-Bell, Lawrence E. Banks, Peter N. Brown, George Byrne, Rujeko Chinomona, Scott D. Cohen, Aaron Collier, Keith E. Grant, Steven L. Lee, Shelby L. Lockhart, John Loffeld, Daniel McGreer, Yu Pan, Slaven Peles, Cosmin Petra, Steven B. Roberts, H. Hunter Schwartz, Jean M. Sexton, Dan Shumaker, Steve G. Smith, Shahbaj Sohal, Allan G. Taylor, Hilari C. Tiedeman, Chris White, Ting Yan, and Ulrike M. Yang.

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nfe	=	3582			
netf	=	150	nsetups	=	436
nni	=	3580	ncfn	=	12
nfSe	=	7164	nfeS	=	14328
netfs	=	0	nsetupsS	=	0
nniS	=	0	ncfnS	=	0

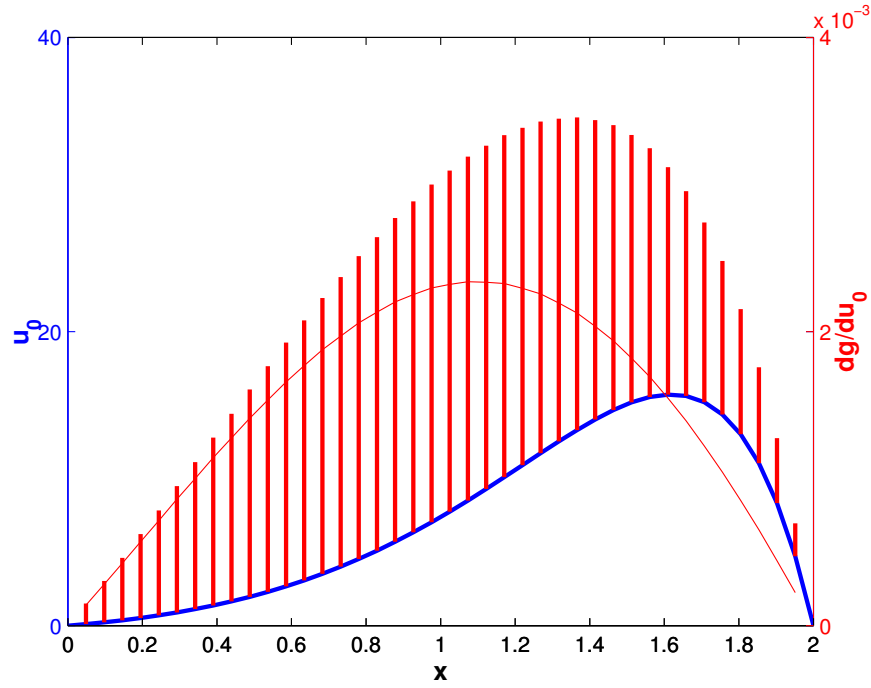


Figure 4: Results for the `cvsAdvDiff_ASAP_non_p` example problem. The gradient of $g(t_f)$ with respect to the initial conditions u_0 is shown superimposed over the values u_0 .

```
[ 2]: -1.097739e-02

mu(t0)
[ 1]: 2.776607e-04
[ 2]: 5.619775e-04
[ 3]: 8.477404e-04
[ 4]: 1.126412e-03
[ 5]: 1.393777e-03
[ 6]: 1.639607e-03
[ 7]: 1.861184e-03
[ 8]: 2.047397e-03
[ 9]: 2.197434e-03
[10]: 2.300275e-03
[11]: 2.357283e-03
[12]: 2.358593e-03
[13]: 2.307827e-03
[14]: 2.197332e-03
[15]: 2.032873e-03
[16]: 1.809960e-03
[17]: 1.536162e-03
[18]: 1.210898e-03
[19]: 8.430003e-04
[20]: 4.362428e-04
```

3.3 A parallel example using CVBBDPRE: `cvsAtmDisp_AS Ai_kry_bbd_p`

As a more elaborate example of a parallel adjoint sensitivity calculation, we describe next the program `cvsAtmDisp_AS Ai_kry_bbd_p` provided with CVODES. This example models an

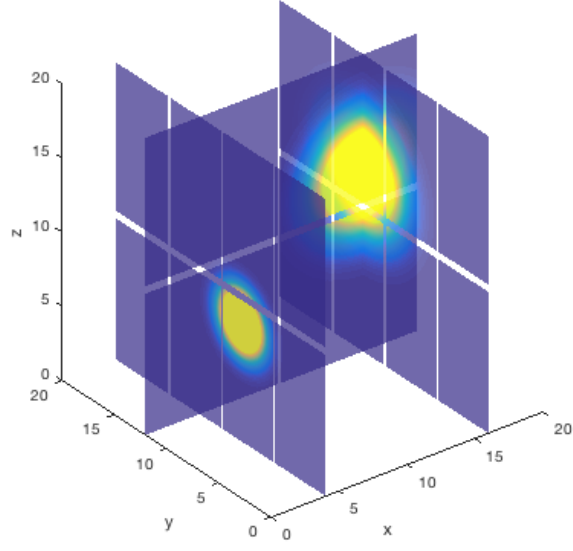


Figure 6: Results for the `cvsAtmDisp_ASai_kry_bbd_p` example problem in 3D. Nominal values of the source parameters.

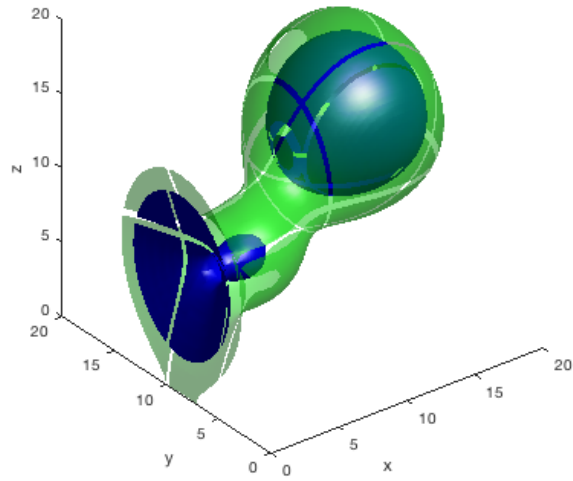


Figure 7: Results for the `cvsAtmDisp_ASai_kry_bbd_p` example problem in 3D. Two isosurfaces of the gradient with respect to the source parameters. They correspond to values of 0.25 (green) and 0.4 (blue).

nst	=	169		
nfe	=	172	nfel	= 303
nni	=	169	nli	= 303
nsetups	=	18	netf	= 0
npe	=	3	nps	= 469
ncfn	=	0	ncfl	= 0

Begin backward integration... done.

Final Statistics..

lenrw	=	150999	leniw	=	236
llrw	=	78786	lliw	=	126
nst	=	119			
nfe	=	135	nfel	=	278
nni	=	132	nli	=	278
nsetups	=	16	netf	=	0
npe	=	3	nps	=	402
ncfn	=	0	ncfl	=	0

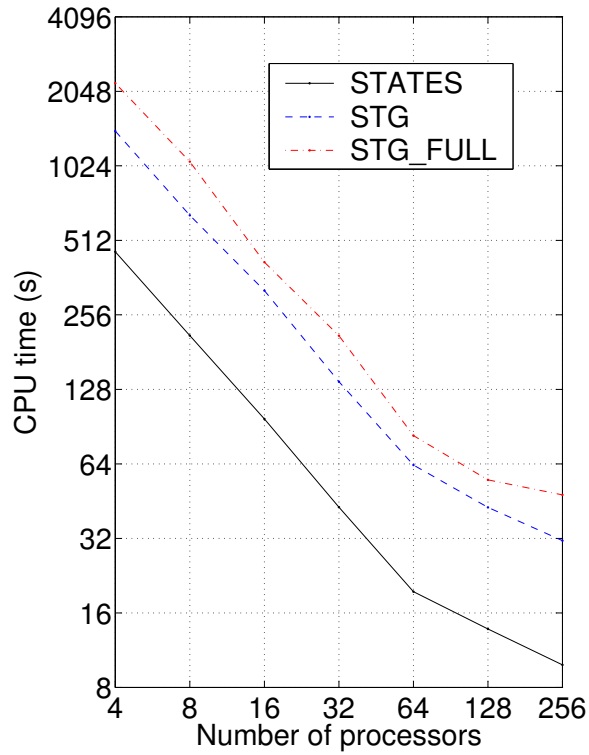


Figure 8: Speedup results for the integration of the state equations only (solid line), staggered sensitivity analysis without error control on the sensitivity variables (dashed line), and staggered sensitivity analysis with full error control (dotted line)

The departure from the ideal line of slope -1 is explained by the interplay of several conflicting processes. On one hand, when increasing the number of processes, the preconditioner quality decreases, as it incorporates a smaller and smaller fraction of the Jacobian, and the cost of interprocess communication increases. On the other hand, decreasing the number of processes leads to an increase in the cost of the preconditioner setup phase and to a larger local problem size which can lead to a point where a node starts memory-paging to disk.

References

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- [4] M. R. Wittman. Testing of PVODE, a Parallel ODE Solver. Technical Report UCRL-ID-125562, LLNL, August 1996.

