**A note on EpiSim speed**

R package EpiSim uses R package deSolve to solve ordinary differential equations corresponding to the model specified in an excel workbook. Many methods are available in deSolve. In EpiSim, deSolve’s method “lsoda” is used (either hardcoded or default depending on the vintage of EpiSim) as it is deSolve’s default/suggested method. The present note indicates that deSolve’s method “ode45” may be better in some circumstances.

This claim is based on the following experiment where workbook “PHAC\_\_m22A-NewFit-v60W1KL-NI.xlsx”[[1]](#footnote-1) is run from time 550 to 800. We tried to do this with 11 different methods as shown in table below.

Results of experiment (start time 2021-11-17 19-42-11)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Method | task | worker | time | Results relative to lsoda |
| 1, lsoda | 11 | 9 | 4.9 hours | reference |
| 2, lsode | 1 | 1 | > 12.5 hours | ?? |
| 3, lsodes | 2 | 1 | ??? 🡪 > 1h40m | ?? |
| 4, lsodar | 3 | 2 | 4.9 hours | Exactly the same |
| 5, vode | 4 | 2 | 4.6 hours | Same if ignore rounding errors |
| 6, daspk | 5 | 3 | > 12.5 hours | ?? |
| 7, euler | 6 | 4 | 1.4 minutes | Substantial differences |
| 8, rk4 | 7 | 5 | 3.7 minutes | Substantial differences |
| 9, ode23 | 8 | 6 | 3.7 minutes | Substantial differences |
| 10, ode45 | 9 | 7 | 40.7 minutes | Same if ignore rounding errors |
| 11, radau | 10 | 8 | > 12.5 hours | ?? |

Random notes

1. Workbook “PHAC\_\_m22A-NewFit-v60W1KL-NI.xlsx” was run from time 550 to 800 with EpiSim 0.12.16.
2. In EpiSim 0.12.16, method may be provided by string (e.g. “vode”) or number (e.g. 5). This is why we show both in the “Method” column.
3. The experiment was done with parallel computing where 11 tasks were submitted to 9 workers. To be sure that lsoda would not be sent to a worker doing something else, it was made the last task (11) handled by the last worker (9). This explain the weird method vs task pattern. This does not matter here hence the light grey fonts. The info is solely provided in case someone needed to revisit the results and parse them correctly.
4. The experiment was started on 2021-11-17 19-42-11 and was killed 12.5 hours later on 2021-11-18 08:09:07. Workers #1, #3 and #8 were still running then. Worker #1 did not dump intermediate results which means that it was still running task 1 (method 2 aka lsode). To figure out how method 3 fared, another experiment was launched on 2021-11-18 10-33-29 where method 3 and 10 were tried. It confirmed that method 10 does indeed take about 40 minutes and it showed that method 3 takes more than 1h40 (it was interrupted).
5. Method 8 and 9 (i.e. rk4 and ode23) give exactly the same results.
6. Method 7, 8 and 9 are fast but give results that are not acceptable (negative values where non-negative expected) as illustrated below

iota = c(550:556,561,seq(581,781,20))

cbind(worker9$df.sweep$time[iota],worker9$df.sweep$vacc1\_S3[iota],worker4$df.sweep$vacc1\_S3[iota], worker6$df.sweep$vacc1\_S3[iota] )

time method1 method7 method9

549 77257.951806 77257.952 77257.9518

550 16969.762624 16969.763 16969.7626

551 148.681047 -42831.461 -8741.3971

552 148.678399 -33997.874 -646.4379

553 148.675375 -25270.828 -26220.2833

554 148.671918 -16676.074 -17666.9122

555 148.667969 -8243.126 -9289.4384

560 179.574929 -32493.750 -1184.4010

580 45.326236 -16586.732 -13625.5021

600 17.956161 -6661.972 -5839.5243

620 18.721128 -5025.910 -4450.0938

640 16.133399 -4333.017 -3835.7763

660 14.278892 -3835.478 -3394.9690

680 12.722504 -3416.747 -3024.9287

700 11.361777 -3050.481 -2701.3948

720 10.156693 -2726.164 -2414.8676

740 9.083824 -2437.497 -2159.7778

760 8.126285 -2179.923 -1932.1107

780 7.270614 -1949.807 -1728.6648

The above speed performance is for a particular workbook ran from time 550 to 800. With the same workbook ran from time 0 to 550, method 1 and 10 (lsoda and ode45) have similar performance (about 20 minutes each). There may be instances where lsoda is indeed preferable to ode45. Brief, one needs to keep in mind this is a case study more than anything else and broad conclusion must be avoided. Do not burn the lsoda bridge yet.

In EpiSim 0.12.16, different deSolve methods are readily assessable via the episim.control argument of seir.n.age.classes function. However, one may be accustomed to work with a previous version EpiSim and thus not willing to embrace a newer version such as 0.12.16. In this case, one will need to hack the seir.n.age.classes function to be able to use method ode45 instead of lsoda. In particular, for very old versions, on may need to change the code in seir.n.age.classes as suggested below.

|  |  |
| --- | --- |
| Old code | output <- lsoda(y = unlist(list.inits),  times = time,  func = calculate\_derivatives,  parms = list.parms,  names.inits = names(list.inits)  ) |
| New  code | output <- deSolve::ode( y = unlist(list.inits),  times = time,  func = calculate\_derivatives,  parms = list.parms,  names.inits = names(list.inits),  method = "ode45" , # "lsoda"  ) |

Appendix

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| R code micro film |
| # Note that was a bug in verbose.save so that the files below contained "object", not "results.this.far"  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 2).SavedFromR"); worker2 =object; rm(object)  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 4).SavedFromR"); worker4 =object; rm(object)  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 5).SavedFromR"); worker5 =object; rm(object)  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 6).SavedFromR"); worker6 =object; rm(object)  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 7).SavedFromR"); worker7 =object; rm(object)  load("M:/UserWorkArea/Claude/PHAC-SEIR/stop/.m22A.N1.runtil800.explore9 2021-11-17 19-42-11/This file contains an R object called results.this.far (worker 9).SavedFromR"); worker9 =object; rm(object)    look.method4 = compare.models( worker2$df.sweep[ seq(801),] , worker9$df.sweep , ignore.vars = "etiquette" ) # same !!!  look.method5 = compare.models( worker2$df.sweep[801+seq(801),] , worker9$df.sweep , ignore.vars = "etiquette" ) # same if ignore rounding errors  look.method7 = compare.models( worker4$df.sweep , worker9$df.sweep , ignore.vars = "etiquette" ) # very different  look.method8 = compare.models( worker5$df.sweep , worker9$df.sweep , ignore.vars = "etiquette" ) # very different  look.method9 = compare.models( worker6$df.sweep , worker9$df.sweep , ignore.vars = "etiquette" ) # very different  look.method10 = compare.models( worker7$df.sweep , worker9$df.sweep , ignore.vars = "etiquette" ) # same if ignore rounding errors  look.method78 = compare.models( worker4$df.sweep , worker5$df.sweep , ignore.vars = "etiquette" ) # Method 7 very different from Method 8 (and 9)  look.method79 = compare.models( worker4$df.sweep , worker6$df.sweep , ignore.vars = "etiquette" ) # Method 7 very different from Method 9 (and 8)  look.method89 = compare.models( worker5$df.sweep , worker6$df.sweep , ignore.vars = "etiquette" ) # Method 8 and 9 are exactly the same  look = look.method10  plot(look$rel.diff.max)  plot(look$diff.max)  plot(look$bad.both)  #subset(look,bad.both>0)  iota = c(550:556,561,seq(581,781,20))  cbind(worker9$df.sweep$time[iota],worker9$df.sweep$vacc1\_S3[iota],worker4$df.sweep$vacc1\_S3[iota], worker6$df.sweep$vacc1\_S3[iota] ) # method 1 versus method 7 versus method 9 |

1. This file is not loaded on the GIT repo as it may be proprietary. It suffices to say that it embodies a model with 236 compartments, each with 6 age groups (so 1416 compartments really). [↑](#footnote-ref-1)