do_steep segfaults with non-interacting system

04/03/2019 05:27 PM - Mark Abraham

Status: Closed
Priority: Low
Assignee: Mark Abraham
Category: mdrun
Target version: 2019.3
Affected version: git master

Description
At [https://gerrit.gromacs.org/#/c/9382/3](https://gerrit.gromacs.org/#/c/9382/3) I accidentally tested something with steepest descent on a system that does not interact. In such cases, the max force is zero, and minimizers should exit gracefully rather than choose a step size based on e.g. dividing by the max force.

Associated revisions
Revision f895f84a - 05/02/2019 09:54 AM - Paul Bauer
Fix FPE in do_steep
Fixes error when running non-interacting system in steepest decent minimization.
Fixes #2917
Change-Id: laff794ab6c2d41e8c4b3d89feefae6ae2372ddf

History
#1 - 04/09/2019 03:51 PM - Mark Abraham
- Target version changed from 2019.2 to 2019.3

This would be nice to fix, but it's such a corner case and has probably been an issue for a long time, so we can leave it for later.

#2 - 05/02/2019 04:30 PM - Paul Bauer
- Status changed from New to Resolved

Applied in changeset f895f84aa9268cd7c636aed1a13b980b1e8a37f.

#3 - 05/03/2019 11:18 AM - Paul Bauer
- Status changed from Resolved to Closed