

Re: Fast solution to very small eigenvalue problem

Source: <http://coding.derkeiler.com/Archive/General/comp.programming/2004-06/1455.html>

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In article <avMcc.131446\$Gx4.109902@bgtnc04-news.ops.worldnet.att.net>, K. Doniger <k.doniger@ieee.org> wrote:

>>

>*If this derives from a physical problem, perhaps you can use Rayleigh's*
>*variational principle.*

The problem involves aligning molecules in 3D. The problem reduces down to constructing a symmetric 4x4 matrix from the atomic coordinates, and the eigenvector corresponding to the largest eigenvalue of that matrix is the rotation quaternion giving the best least-squares fit (see http://www.osc.edu/PET/CCM/skeleton/software/tested/source/qtrfit/qtrfit_theory.html, with the caveat that the matrix is depicted wrongly: it is actually symmetric)

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Mark Mackey

"The determined Real Programmer can write Fortran programs in any language."
- "Real Programmers don't use Pascal"