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Gaussian 16 expands the range of molecules and types of chemical problems that you can model. More...

Gaussian.com | Expanding the limits of computational chemistry

Hi Harish! Wow, your question is not a short one! Basically Gaussian uses the Berny Optimization algorithm which calculates all forces on every atom (i.e. which way and how strongly is each atom being pushed or pulled by the rest of the atoms) then it also calculates the gradient of such forces and allows them to be pushed -or pulled- just a ...

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In statistics, originally in geostatistics, kriging or Gaussian process regression is a method of interpolation for which the interpolated values are modeled by a Gaussian process governed by prior covariances.

Kriging - Wikipedia

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Vacuum permittivity - Wikipedia

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