Computational Materials Physics

Center for Molecular Modeling

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functions and functionals

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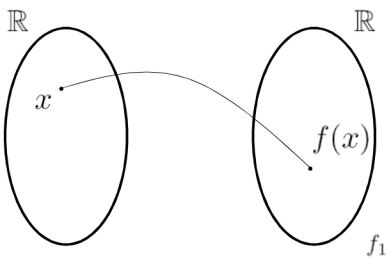
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

function

$$f : \mathbb{R} \mapsto \mathbb{R} : x \mapsto f(x)$$



$$\begin{aligned} f_1(x) &= 5x + 2 \\ f_2(x) &= 3x^2 - 7x + 6 \\ f_3(x) &= e^x \end{aligned}$$

functional

A **function** maps *numbers* onto (complex) numbers :

$f : \mathbb{R} \to \mathbb{R} : x \mapsto f(x)$ $\qquad$ $f : \mathbb{C} \to \mathbb{C} : x \mapsto f(x)$

A **functional** maps *functions* onto (complex) numbers :

$F : \mathcal{F} \to \mathbb{C} : f \mapsto \mathcal{F}[f]$

Examples : $F[f] = \int_{-\infty}^{\infty} f(x) e^{-x^2} dx$

$F[f] = f(0)$

Functional derivative: generalization of derivative for functions.

Example: $F_v[\rho] = \int \rho(\vec{r}) v(\vec{r}) d\vec{r}$

$\frac{\delta F_v[\rho]}{\delta \rho} = v(\vec{r})$