Mitglied der Helmholtz-Gemeinschaft

JÜLICH FORSCHUNGSZENTRUM

Integration of Higher Order Compact Scheme into Multigrid

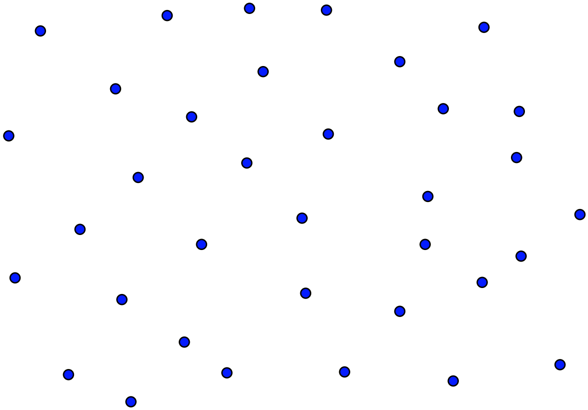
Guest Student Program in Scientific Computing

September 30, 2010 | Alina Istrate adviser: Godehard Sutmann

Outline

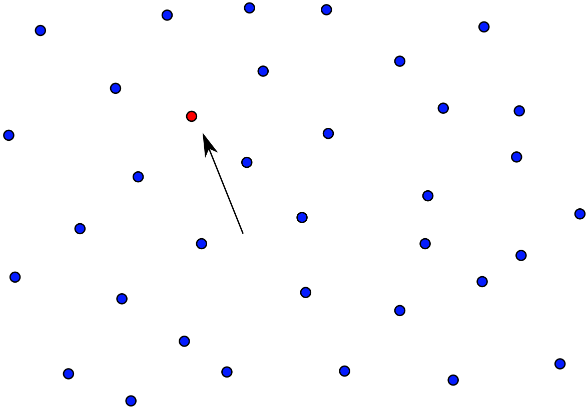
- Introduction to the physics of the problem
- VERY brief introduction to the mathematics of the problem
- Results
- Conclusion
- Outlook

Let there be particles...



Let there be particles...

Particle properties: position, velocity and charge



Basic incredients for Particle Simulation

Given

initial state $S_0 = [\vec{x}_1, ..., \vec{v}_1, ...]$ of a set $\mathcal{P}$ of particles.

Time evolution is given by Newton's equations of motion

$$\vec{v}_i = \frac{d}{dt}\vec{x}_i \qquad \vec{F}_i = \frac{d}{dt}m_i\vec{v}_i$$

The force acting on particle i

$$\vec{F}_i = \sum_{j \in \mathcal{P}/\{i\}} \vec{F}_{i,j}$$

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About potentials

Forces are given by the gradient of the potential

$$\vec{F}_i = -\nabla\Phi_i \qquad \vec{F}_{i,j} = -\nabla\Phi_{i,j} \qquad \Phi_i = \sum_{j\in\mathcal{P}/\{i\}} \Phi_{i,j}$$

Classification

- short range: decays faster than $\frac{1}{r^d}$: Van der Waals potential, Lenard-Jones potential
- long range: decays slower $\frac{1}{r^d}$: Coulomb potential, gravitational potential

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Important definitions

- Coulomb potential

$$\Phi_{i,j} = \frac{1}{4\pi\epsilon_0} \frac{q_j}{\|\vec{x}_i - \vec{x}_j\|_2}$$

- Force

$$\vec{F}_i = \frac{1}{4\pi\epsilon_0} \sum_{j \in \mathcal{P}/\{i\}} q_i q_j \frac{\vec{x}_i - \vec{x}_j}{\|\vec{x}_i - \vec{x}_j\|_2^3}$$

- Electrostatic energy

$$E = \frac{1}{2} \sum_{i \in \mathcal{P}} q_i \Phi_i = \frac{1}{2} \sum_{i \in \mathcal{P}} q_i \sum_{j \in \mathcal{P}/i} \frac{q_j}{\|\vec{x}_i - \vec{x}_j\|_2}$$

Properties of the system

Important definitions

- Coulomb potential

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How to simulate a particle system

Important

In our system the particles are interacting by Coulomb force!

What we need to do

- Calculate the forces at the current time
- Use a time integration scheme to move to the next time step

Definition

Integration scheme is a ”magical” tool which needs as input at least the forces and the velocities at one time step and they provide the new positions and updated velocities as output

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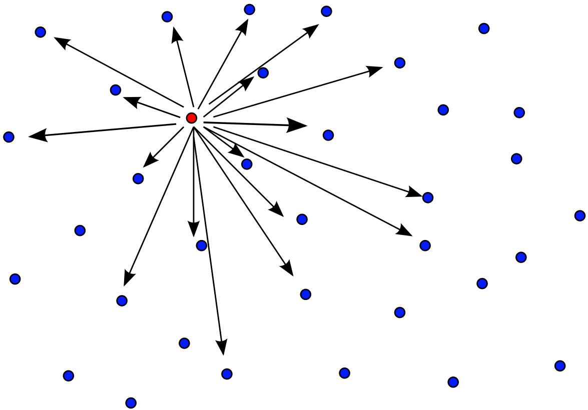
How do we get the forces?

Like always, several approaches exist!

How do we get the forces?

Particle-Particle Methods



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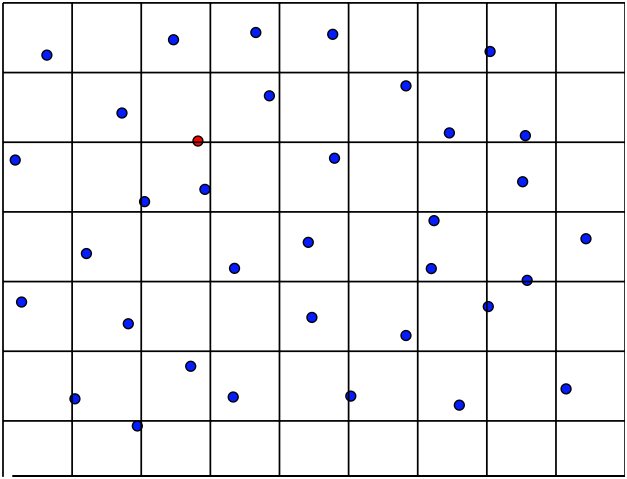
Particle-Mesh Methods



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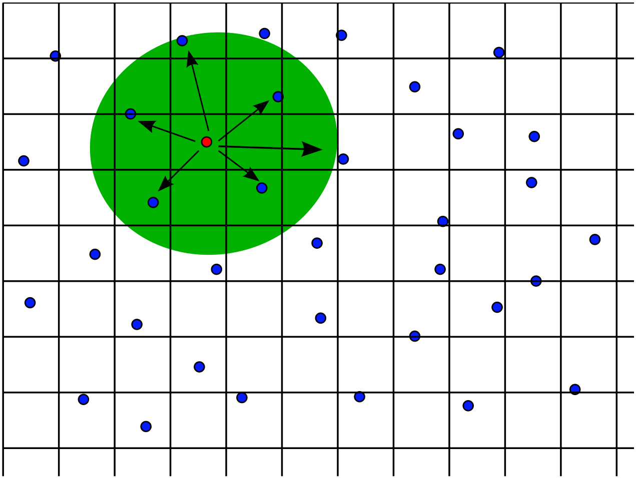
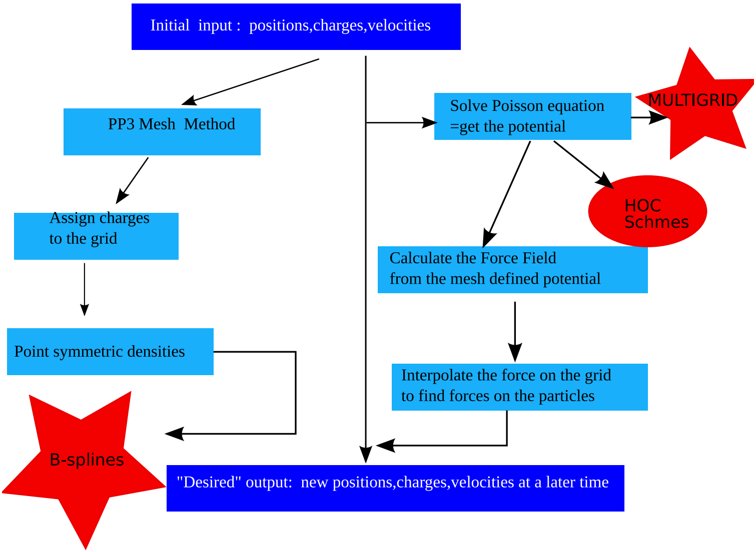
Particle-Particle-Particle Mesh Methods



General view



Relation to Poisson equation

Green's function of the Poisson equation in $\mathbb{R}^3$

$$U(x) = \frac{1}{4\pi\|\vec{x}\|_2}$$

Reminder: Coulomb potential

$$\Phi_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{1}{4\pi\epsilon_0} \frac{q_j}{\|\vec{x}_i - \vec{x}_j\|_2}$$

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Arriving at the starting point...

Coulomb potential is a solution of the Poisson equation

$$\Delta\Phi_i(\vec{x}) = \rho_i := \frac{1}{\epsilon_0}\sum_{\substack{j=1 \\ j\neq i}}^{N} q_i\delta(\|\vec{x}_i - \vec{x}_j\|_2)$$

- This is the potential induced by all particles except for the i-th particle
- Can not straightforwardly be solved numerically
- define numerical schemes to calculate the electrostatic quantities of the system based on the solution of the Poisson equation on a mesh

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Meshed Continuum Method

- Unlike other PP-PM methods the current approach uses a continuum description: not assigning point charges to the grid but replace the point charges by charge distribution
- Do not introduce additional discretization errors

Solution

- Replace δ distribution on right hand side by

$$\rho_g = g(\|x\|_2)$$

  with the properties:
  - g:$\mathbb{R}_0^+ \rightarrow \mathbb{R}_0^+$
  - g is sufficiently smooth
  - $\int_{\mathbb{R}^3} \rho_g(x) = 1$
  - solution Φ_g of $-\Delta\Phi_g(x) = \frac{1}{\epsilon_0}\rho_g(x)$ is known analytically
- g must have a limited support, i.e.

$$g(x) = 0 \text{ for x} > \text{R}$$

Point symmetric densities described by B-splines

Definition

A B-spline B_i, $i = 0, 1, ...$ of unit width is given by

$$B_0 = \begin{cases} 1, & -\frac{1}{2} \leq x \leq \frac{1}{2} \\ 0, & otherwise \end{cases}$$

$$B_{i+1}(x) = 2B_{[i/2]}(2x) * 2B_{i/2}(2x), \text{ for } i = 1, 2...$$

"Simple" example:

4th order B-spline

$$\rho_{B_4}(r) = \begin{cases} \frac{27\cdot(81\cdot r^4 - 54\cdot r^2\cdot R^2 + 11\cdot R^4)}{32\cdot R^7} & r \leq \frac{R}{3} \\ \frac{27\cdot(-9\cdot r^2 + 6\cdot r\cdot R + R^2)(27\cdot r^2 - 42\cdot r\cdot R + 17\cdot R^2)}{64\cdot\pi\cdot R^7} & r \leq \frac{2R}{3} \\ \frac{2187\cdot(r - R)^4}{64\cdot\pi R^7} & r \leq R \end{cases}$$

Remark

The analytical solution for the potential energy is known

Back to 3D Poisson equation

$$\nabla^2 \Phi = f$$

$$\nabla^2 = \frac{\partial^2}{\partial x} + \frac{\partial^2}{\partial y} + \frac{\partial^2}{\partial z}$$

How to implement the Laplacian on the computer?

Answer: Finite differences

Finite differences in one dimension

Definition

Derivative of a function is defined by the difference quotient

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

The discretization of a derivative on a equispaced grid with grid width h is:

$$f'(x) \doteq \frac{f(x+h) - f(x)}{h}$$

Using Taylor expansion the error is found to be $\mathcal{O}$(h)

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Finite differences in one dimension

Example

The second order derivative

$$f'' = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + \mathcal{O}(h^2)$$

Higher order approximations can be constructed by using more grid points, e.g. not only $x - h$, x and $x + h$, but $x - 2h$, $x + 2h$,...

1D analogue of the Poisson equation

Example

for periodic boundary conditions

$$u''(x) = f(x)$$

$$\begin{cases} \frac{1}{h^2}(u_n - 2u_0 + u_1) = f_0 \\ \frac{1}{h^2}(u_{i-1} - 2u_i + u_{i+1}) = \quad f(x) \quad \text{for } i = 1, ..., n-1 \\ \frac{1}{h^2}(u_n - 2u_0 + u_1) = f_0 \end{cases}$$

with $u_i = u(ih)$, $f_i = f(ih)$

The system can be solved with multigrid method

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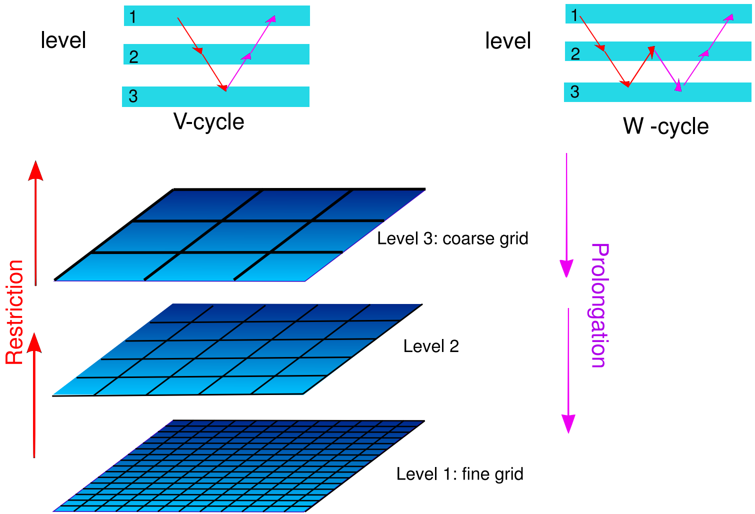
Very short introduction to Multigrid



Finite differences for higher dimensions

2D

$$\Delta u(\vec{x}) = \frac{1}{h^2}[u(\vec{x} - h\vec{e}_1) + u(\vec{x} - h\vec{e}_2) - 4u(\vec{x}) + u(\vec{x} + h\vec{e}_1) + u(\vec{x} + h\vec{e}_2)] + \mathcal{O}(h^2)$$

Stencil notation

$$\frac{1}{h^2}\begin{bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{bmatrix}$$

Finite differences for higher dimensions

3D

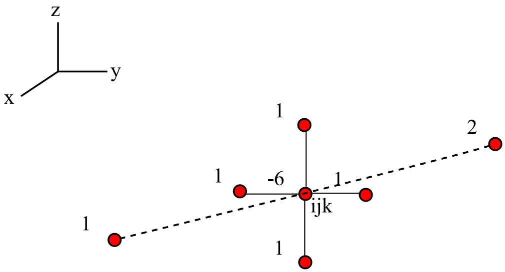
$$\Delta u(\vec{x}) = \frac{1}{h^2}[u(\vec{x} - h\vec{e}_1) + u(\vec{x} - h\vec{e}_2) + u(\vec{x} - h\vec{e}_3) - 6u(\vec{x}) + u(\vec{x} + h\vec{e}_1) + u(\vec{x} + h\vec{e}_2) + u(\vec{x} + h\vec{e}_2)] + \mathcal{O}(h^2)$$

Stencil notation

$$\frac{1}{h^2}\begin{bmatrix} & & \\ & 1 & \\ & & \end{bmatrix} \quad \frac{1}{h^2}\begin{bmatrix} & 1 & \\ 1 & -6 & 1 \\ & 1 & \end{bmatrix} \quad \frac{1}{h^2}\begin{bmatrix} & & \\ & 1 & \\ & & \end{bmatrix}$$

Stencil representation

2nd order



Simplifying the things...

- $u_{i,j,k} \equiv$ value of u at grid point $\vec{x}_{i,j,k}$
- $f_{i,j,k} \equiv$ value of f at grid point $\vec{x}_{i,j,k}$
- $\partial^2_{x_1} u_{i,j,k}$ being the central finite difference approximation to the second partial derivative in x-direction

Definition

$$\partial^2_{x_1} u_{i,j,k} = \frac{u(\vec{x}_{i-1,j,k}) - 2u(\vec{x}_{i,j,k}) + u(\vec{x}_{i+1,j,k})}{h^2}$$

$$\Delta u_{i,j,k} = \partial^2_{x_1} u_{i,j,k} + \partial^2_{x_2} u_{i,j,k} + \partial^2_{x_3} u_{i,j,k} + \mathcal{O}(h^2)$$

Compact discretization of higher order

Definition

Compact discretization of higher order are discretizations which are taking into account all nearest neighbours, not only the direct ones. Advantage:

- they achieve higher order, but only nearest neighbours are needed
- reduced amount of communication for parallel solvers

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Higher order compact discretization

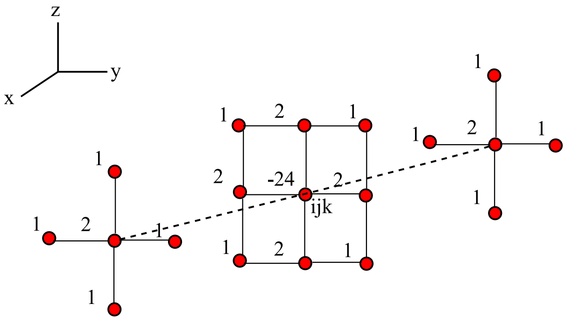
4th order compact scheme

$$[\partial^2_{x_1} + \partial^2_{x_2} + \partial^2_{x_3} + \frac{h^2}{6}(\partial^2_{x_1}\partial^2_{x_2} + \partial^2_{x_1}\partial^2_{x_3} + \partial^2_{x_2}\partial^2_{x_3})]u_{i,j,k} =$$

$$f_{i,j,k} + \frac{h^2}{12}\left[\delta^2_{x_1} + \delta^2_{x_2} + \delta^2_{x_3}\right] f_{i,j,k} + \mathcal{O}(h^4)$$

Stencil representation

4th order



Higher order compact discretization

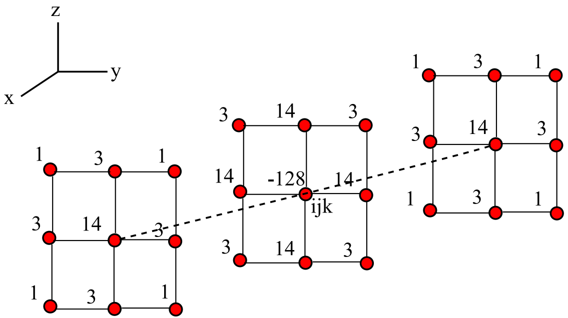
6th order compact scheme

$$[\partial^2_{x_1} + \partial^2_{x_2} + \partial^2_{x_3} + \frac{h^2}{6}(\partial^2_{x_1}\partial^2_{x_2} + \partial^2_{x_1}\partial^2_{x_3} + \partial^2_{x_2}\partial^2_{x_3}) + \frac{h^4}{30}\partial^2_{x_1}\partial^2_{x_2}\partial^2_{x_3}]\Phi_{i,j,k} =$$

$$f_{i,j,k} + \frac{h^2}{12}\nabla^2 f_{i,j,k} + \frac{h^4}{360}\nabla^4 f_{i,j,k} + \frac{h^4}{180}[\frac{\partial^4 f}{\partial x_1^2 \partial x_2^2} + \frac{\partial^4 f}{\partial x_2^2 \partial x_3^2} + \frac{\partial^4 f}{\partial x_1^2 \partial x_3^2}] + \mathcal{O}(h^6)$$

Stencil representation

6th order



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Right hand side of Poisson equation in our case

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Case study

Eigenfunctions of Laplace operator

- source term distribution

$$f_{i,j,k} = 12\pi sin(2\pi i h_x) sin(2\pi j h_y) sin(2\pi k h_z)$$

- with the analytical solution

$$u_{i,j,k} = sin(2\pi i h_x) sin(2\pi j h_y) sin(2\pi k h_z)$$

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Eigenfunctions of Laplace operator

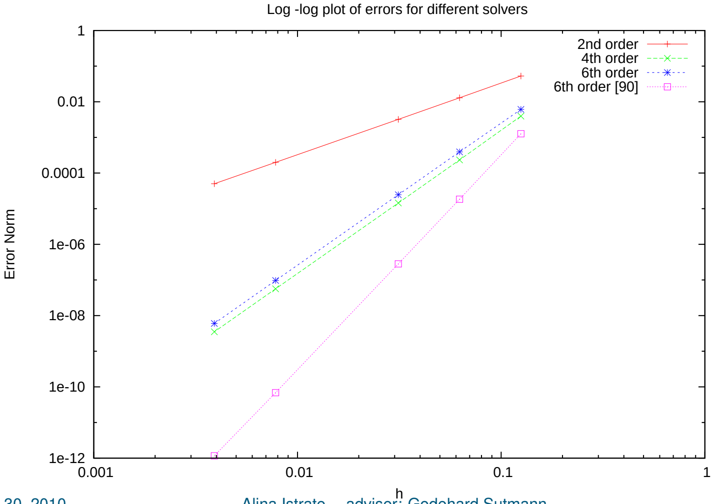
- source term distribution

$$f_{i,j,k} = 12\pi sin(2\pi i h_x) sin(2\pi j h_y) sin(2\pi k h_z)$$

- with the analytical solution

$$u_{i,j,k} = sin(2\pi i h_x) sin(2\pi j h_y) sin(2\pi k h_z)$$

Results



Log -log plot of errors for different solvers
2nd order
4th order
6th order
6th order [90]
Error Norm
h
1
0.01
0.0001
1e-06
1e-08
1e-10
1e-12
0.001
0.01
0.1
1

Conclusions

What I had to do...and what I have done

- implement the 6th order compact scheme into the PP3MG code
- the result is not as expected; possible cause: the 4th order B spline is not enough ”smooth“ when applying the 6th order operators
- measurements of time spent in ”creating“ the left and right hand sides of Poisson equation were done but they were not concludent

Outlook

- implementation of higher order B-spline
- performance gain by combining different HOC schemes hierarchly
- implementation of different 6th order HOC's
- parallel performance measurements

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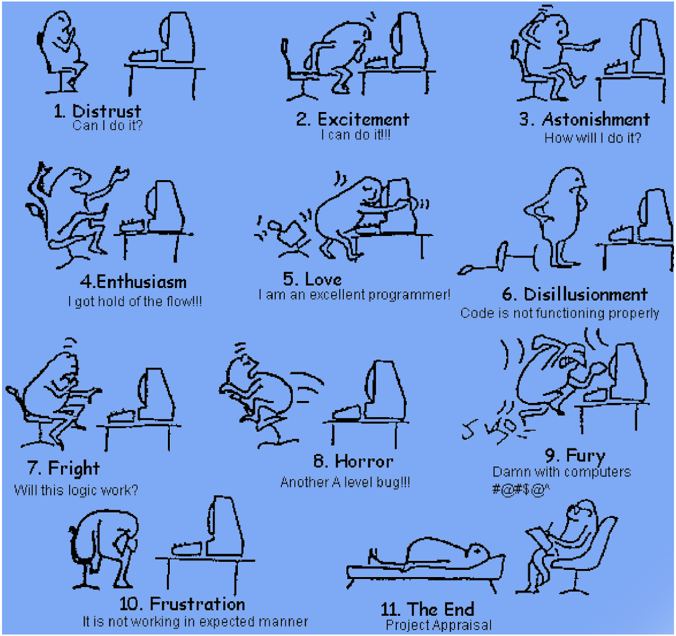
Before... in Experimental Physics

Subject-project interaction diagram



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