

# An outsider looks at SAGE ...

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- Scientific computing person's interest in SAGE
- Computational efficiency in scientific computing
- Casual user's experience and possible project aims

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Talk given ~ 2 weeks ago ...

# Numerical Methods for the Design of 2-Well Quantum Devices

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## Collaborators

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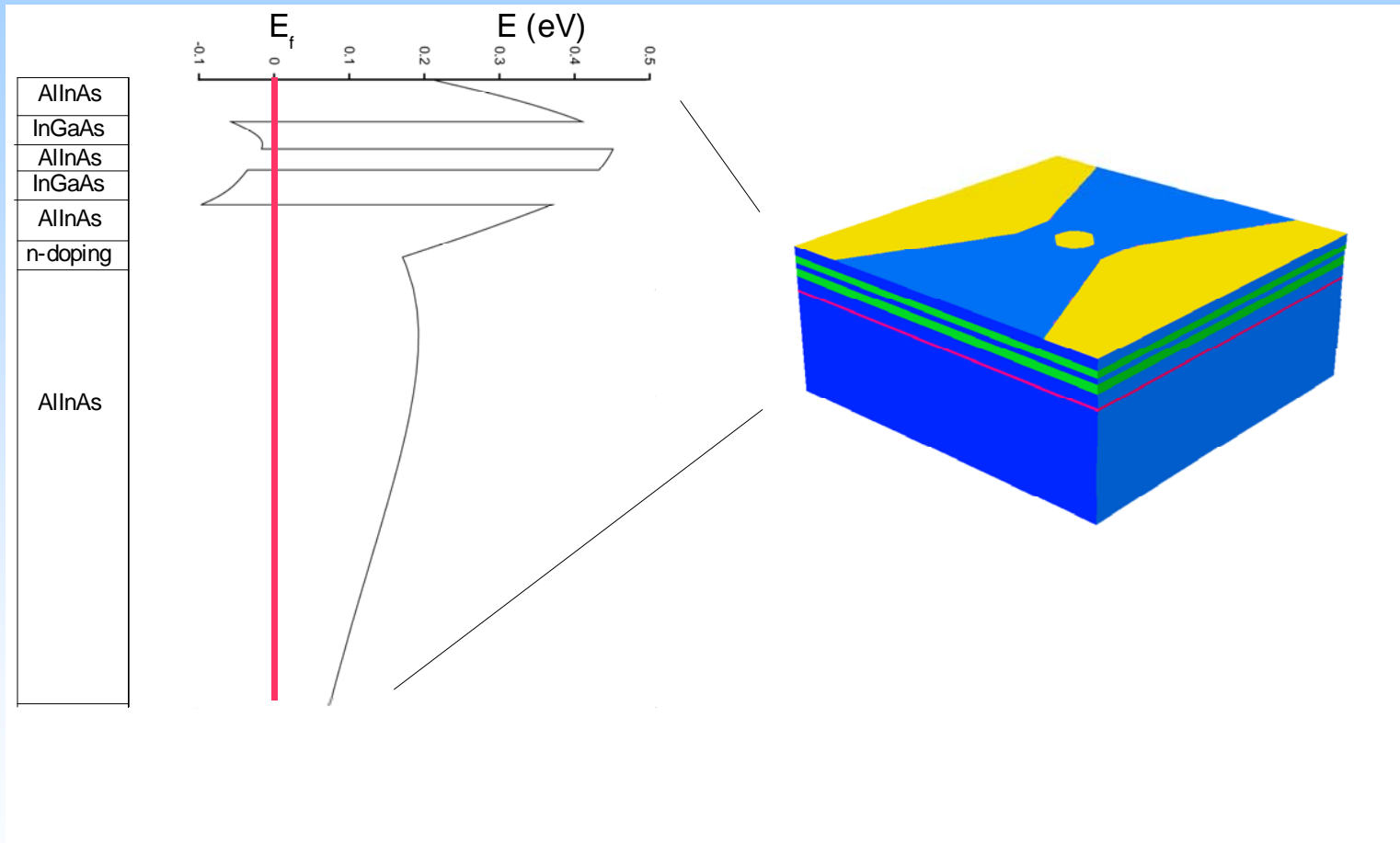
UCLA EE:

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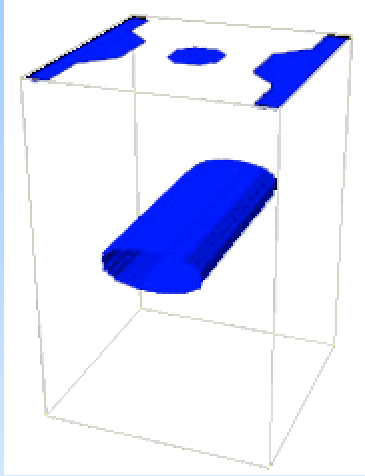
Hans Robinson



# The Target Device:



## Device operation (conceptual):

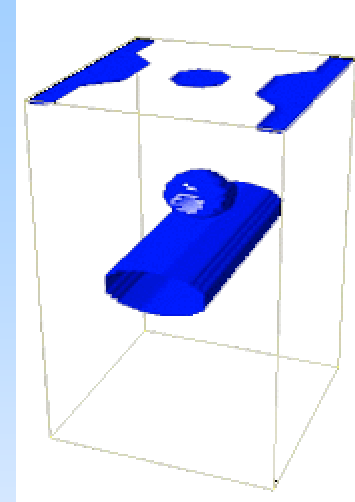


Side voltage applied



quantum wire

Multiple states in the lower well.  
Confinement in 2 directions.



Side and dot voltage applied

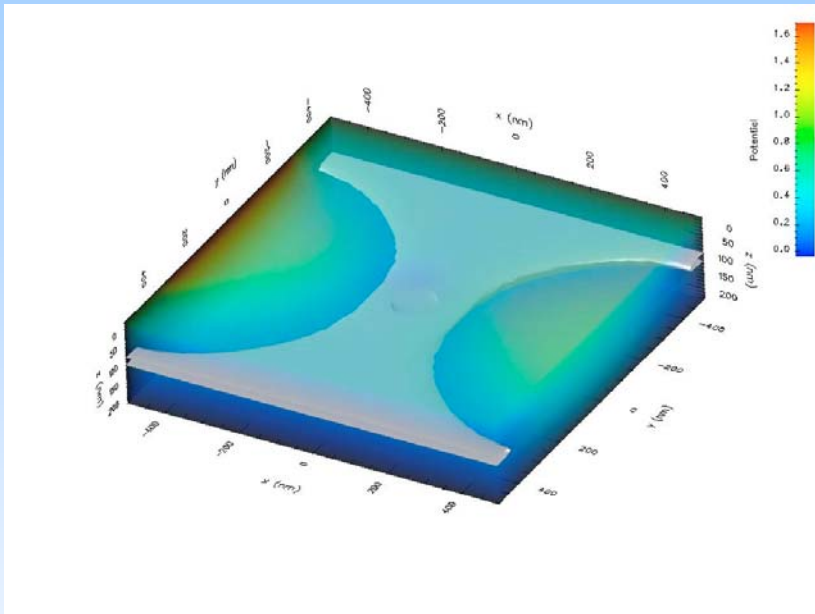


quantum wire + quantum dot

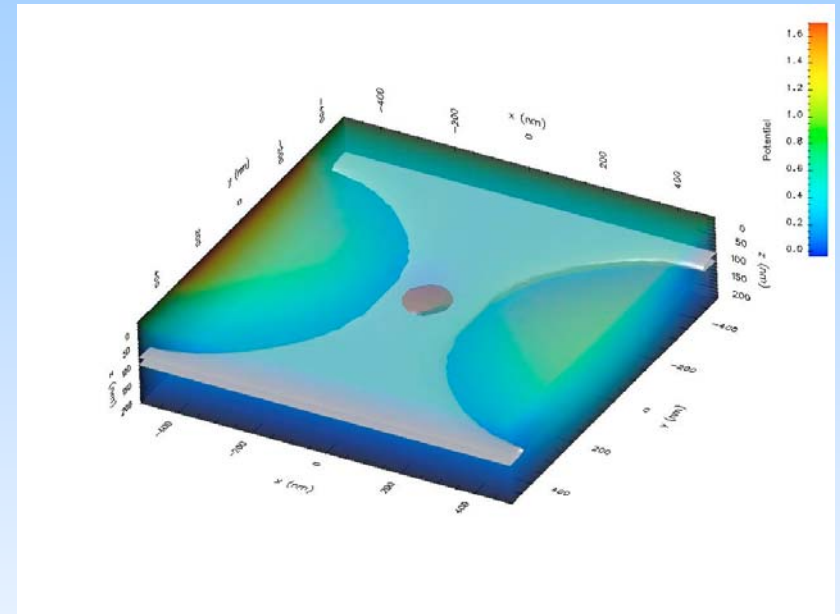
Single state in the upper well.  
Confinement in 3 directions

Multiple states in the lower well.  
Confinement in 2 directions

# Simulation Results:

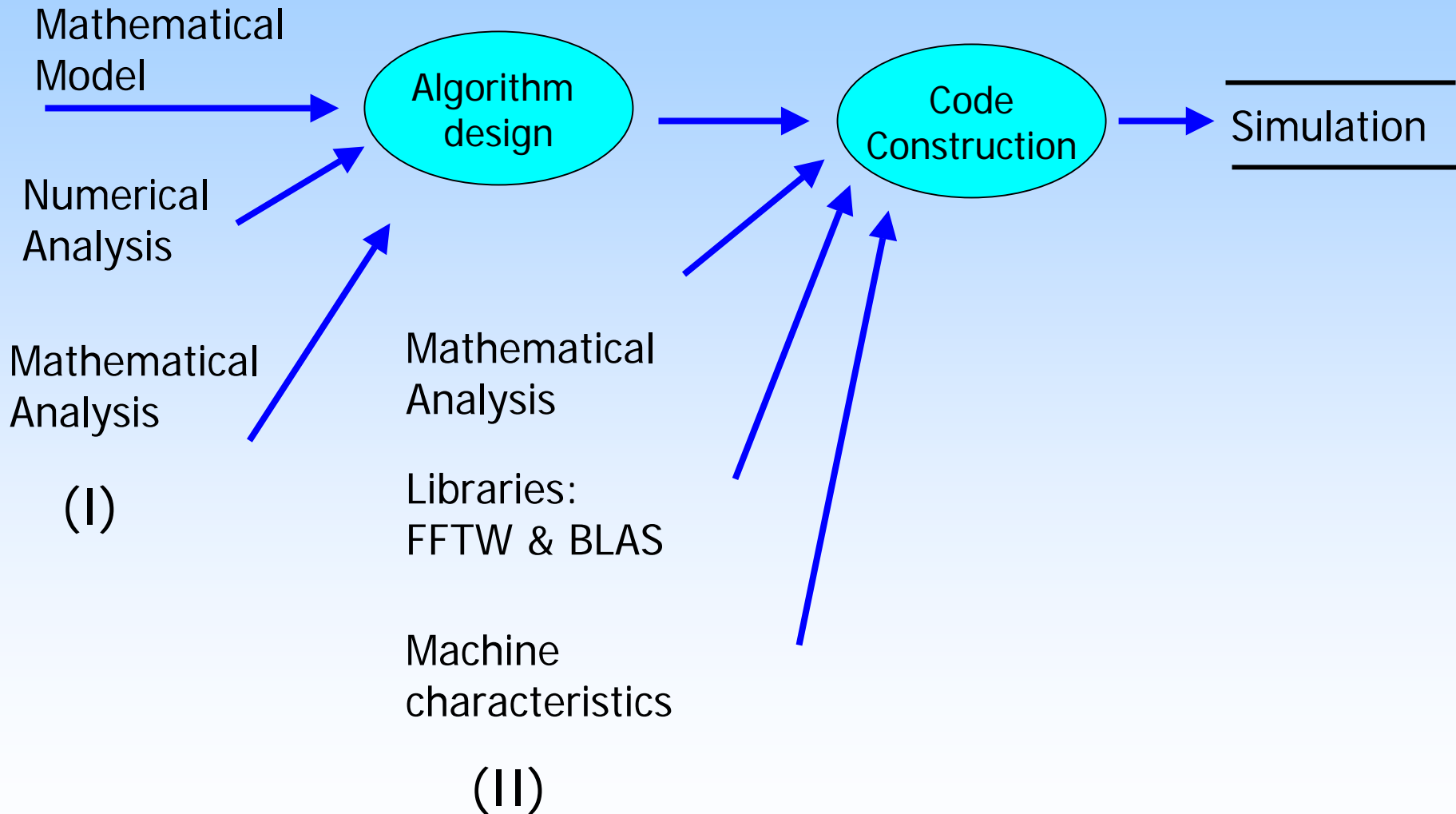


Quantum wire



Quantum wire  
+  
Quantum dot

# Simulation development process

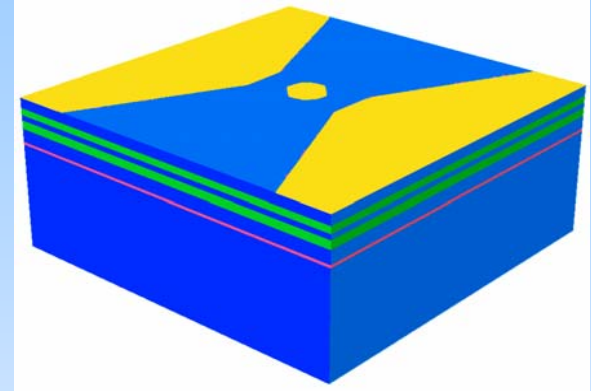


# Simulation development process (I)

$$\nabla \cdot (\varepsilon \nabla \phi) = f(x,y,z)$$

Aspects:

- 3D
- Discontinuous coefficients
- Thin layers
- Non-trivial geometry



Use “analytic” x 2D Fourier basis:

$$\phi(z, x, y) = \sum_{k_1, k_2} a_{k_1, k_2}(z) e^{ik_1 \frac{x}{dX}} e^{ik_2 \frac{y}{dY}}$$

2D Fourier transform at each  $z \Rightarrow$

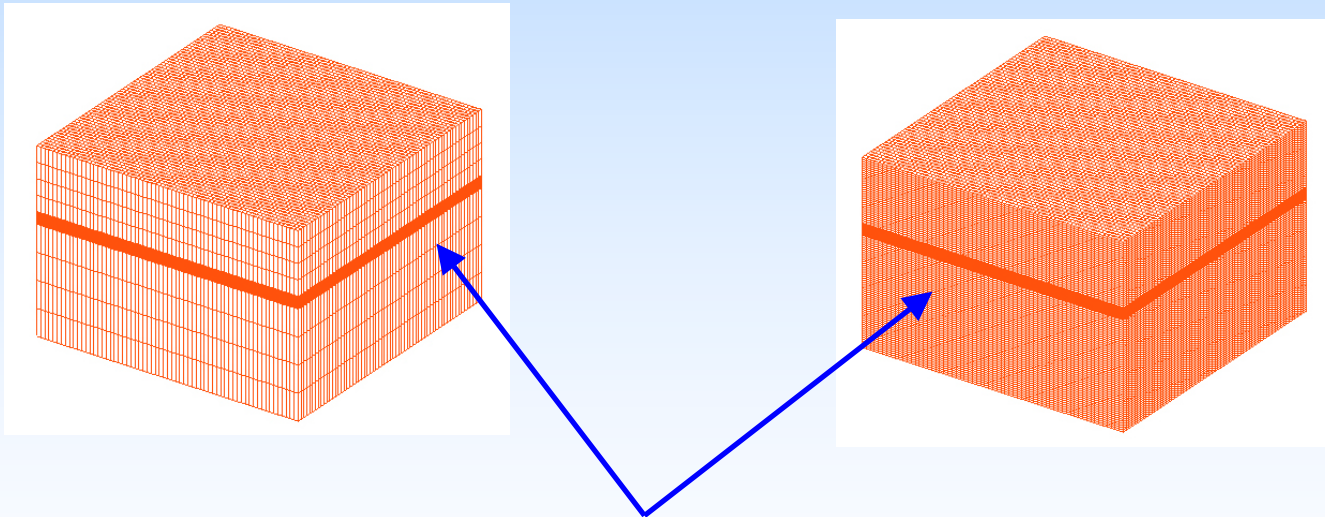
$$\frac{d}{dz} \left( \epsilon \frac{da_{k_1, k_2}(z)}{dz} \right) - \left( \frac{4\pi k_1^2}{dX^2} + \frac{4\pi k_2^2}{dY^2} \right) a_{k_1, k_2}(z) = \hat{f}_{k_1, k_2}(z)$$

Use piecewise analytic solution of 1D equation (extension of Wachspress's idea) and analytic inclusion of  $\delta$  function sources.



# Features

- Exact in harmonic regions
- Allows extreme refinement in z-direction
- High accuracy
- Non-iterative & “Fast”  $O(N_z N_x N_y \log(N_x N_y))$

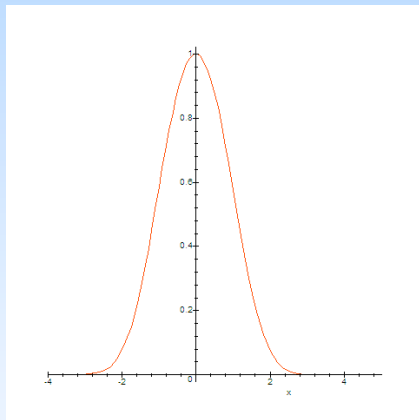


*Equivalent accuracy near wells, even with “extreme” coarsening in the vertical direction.*

# Simulation development process (II)

Analytic formulas can require transformation...

$$f(x) = x^2 / (e^{x^2} - 1)$$



x	f(x)
1.0000000000e-001	5.8197670687e-001
1.0000000000e-002	9.9500833332e-001
1.0000000000e-003	9.9995000083e-001
1.0000000000e-004	9.9999950000e-001
1.0000000000e-005	9.9999999500e-001
1.0000000000e-006	9.9999999966e-001
1.0000000000e-007	1.0000000040e+000
1.0000000000e-008	9.9999696824e-001
1.0000000000e-009	1.0003657307e+000
1.0000000000e-010	1.0248191152e+000
1.0000000000e-011	1.#INF000000e+000
1.0000000000e-012	1.#INF000000e+000
1.0000000000e-013	1.#INF000000e+000
1.0000000000e-014	1.#INF000000e+000

$$f(x) = 1 - x^2/2 + x^4/12 + O(x^8)$$

## Simulation development process (II)

Development of approximations.

$$\frac{d^2 f}{dx^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + (D^{(2)})(f)(x)h^2 + \frac{1}{12}(D^{(4)})(f)(x)h^4 + \frac{1}{360}(D^{(6)})(f)(x)h^6 + \frac{1}{20160}(D^{(8)})(f)(x)h^8 + O(h^{10})$$

$$\frac{d^2 f}{dx^2} = ? + O(h^4)$$
$$? + O(h^6)$$
$$? + O(h^8)$$

## Interest in SAGE

- Formula derivation
- Formula analysis
- Formula transformation for numerical stability w.r.t. finite precision arithmetic and for efficiency
- Other possibilities: e.g. symbolic model identification:

Audoly, S., D'Angio, L., Saccomani, M.P. & Cobelli, C. Global identifiability of linear compartmental models--a computer algebra algorithm. *IEEE Trans Biomed Eng* **45**, 36-47 (1998).

(Search : Audoly + identifiability)

## Why a particular interest in SAGE?

New:

- being created with “new” aims.
- being created by a different collection of people
- being created using “newer” software constructs

Alternate ways of accessing functionality

“A mathematical primordial soup”

Computational efficiency in scientific computing?

# Efficiency techniques in scientific computation

- Mathematical Analysis
- Write procedures in terms of “primitives” whose implementation can be (or is) optimized.

FFTW for Fourier-Transforms\*

Basic Linear Algebra Subroutines (BLAS)

$$\left\{ \begin{array}{l} w \leftarrow A v \\ x \leftarrow \alpha x + y \\ C \leftarrow A^* B \\ \dots \end{array} \right.$$

Automatically Tuned Linear Algebra Subroutines (ATLAS)  
(search ATLAS + BLAS)

\*with appropriate size selection

## Efficiency comments

- Memory access time can be significant.
- Optimizing compilers are good: but one has to avoid code constructs that inhibit optimization.
- Profiling code (detailed code timing) has been invaluable.
- Common sense -- 100000% speed up of code that accounts for 1% of the total computation time will give less than 1% improvement.

### Current problem:

How to take advantage of multi-core processors.



Casual user first impressions and possible project “targets”

Try it out.

How far can I get doing the things that I want to do without external help?

As a "casual" user.

As a "hacker" using SAGE API.

If I had time ...

As a "hacker": Sage API

Exploratory investigation:

Can I get SAGE (or some part of it) to provide the "backend" symbolic functionality for web based applications communicating via XML?

## As a "casual" user

Exploratory tasks:

Installation (PC)

Taylor series expansions

Plotting

Truncation error analysis

Notes/Comments + possible project "targets"

## Installation PC : cygwin + pre-built binaries

It worked. No "hitches"

### Comments:

cygwin → "limited" distribution  
windows users  $\cap$  Unix users

"All in one" → 1/2 GB (w.o. cygwin)

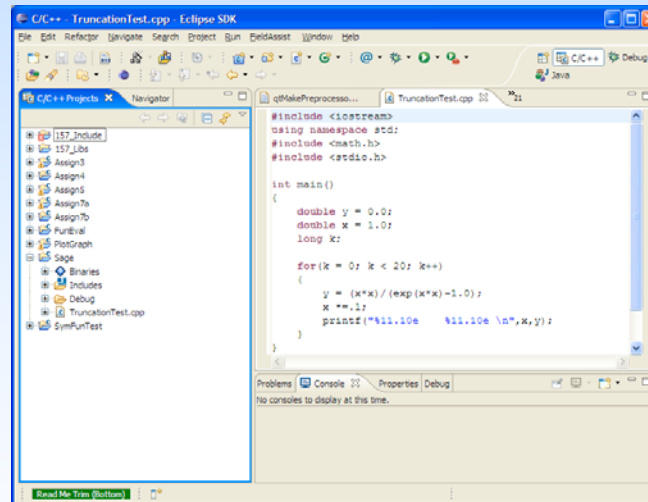
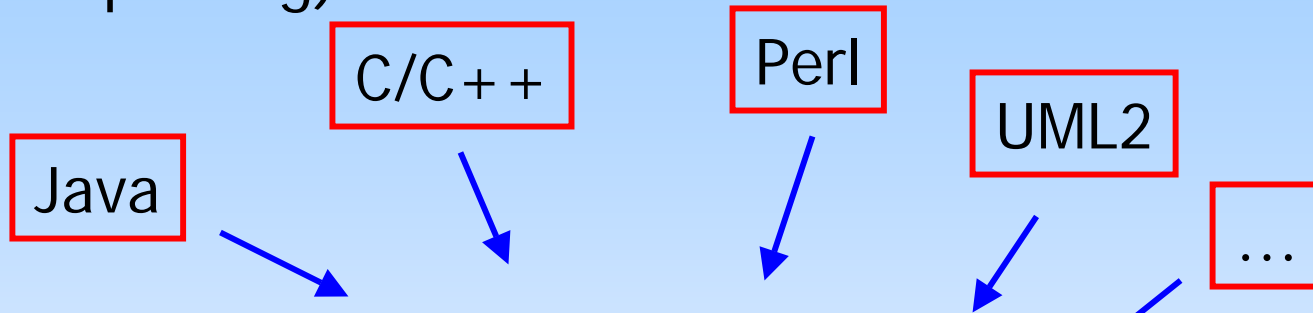
Updates require re-installation?

### Possible project target:

Mimic Eclipse method of distribution and updates...

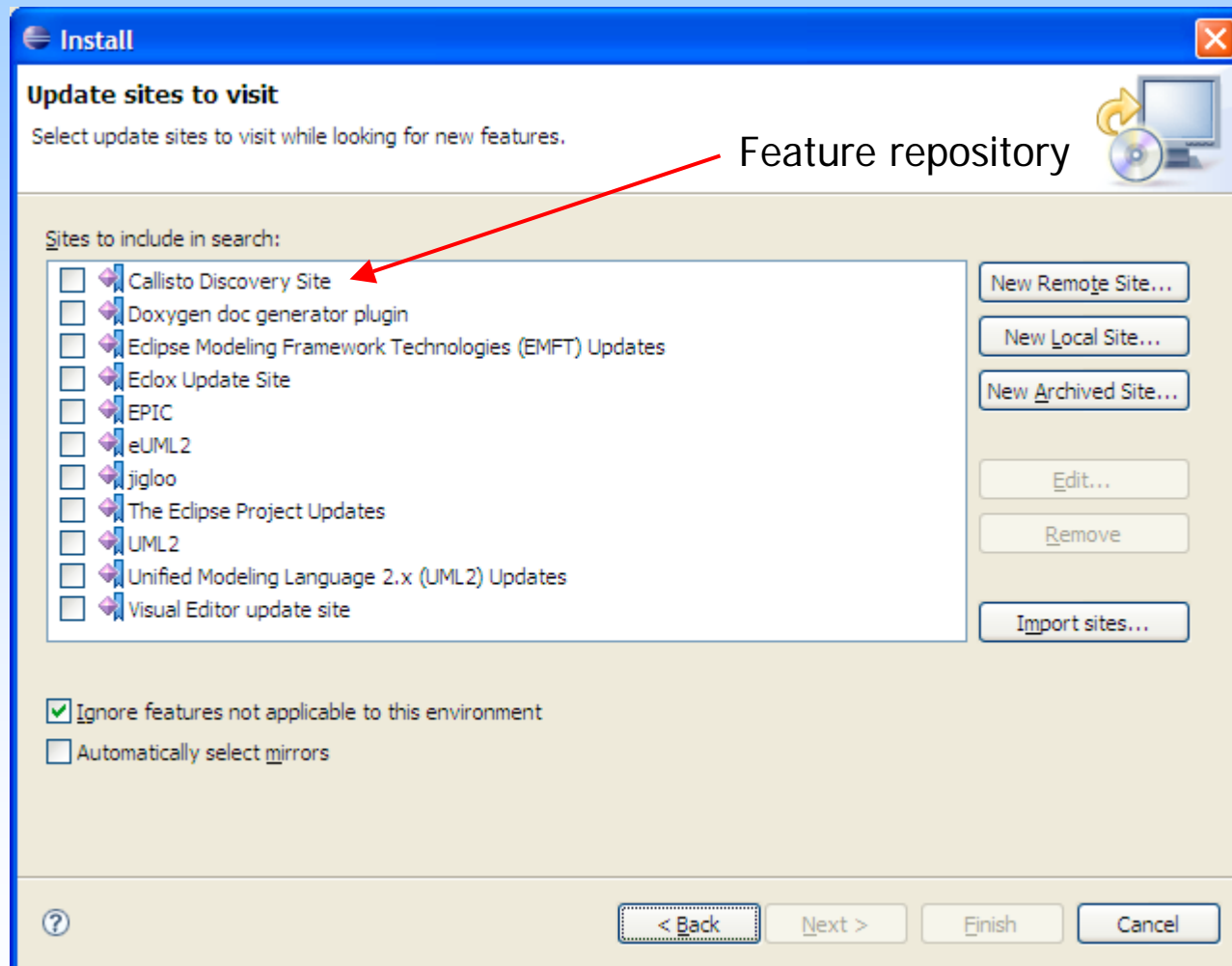
# Eclipse?

Extensible Integrated Development Environment (IDE)  
([www.eclipse.org](http://www.eclipse.org))



# Eclipse Installation Step 1: Install base package + Java

# Eclipse Installation Step 2: Select features and check updates



## Taylor series expansions

### Success.

```
maxima.taylor('x^2/(exp(x^2)-1)', 'x', 0, 10)
```

$$1 - x^2/2 + x^4/12 - x^8/720$$

### Comments:

- Ahh ... green bar means executing  
... it stacks "evaluation" requests.
- It took a while to find the right Maxima function.
- I was only able to figure out what to do by following an example.
- Reference: how to search for a key word?
- Maxima help requires "translation"



## Possible project targets:

Better organized help? Searchable Reference.

Ability to export C/C++ or Java (e.g. not Lisp) code implementing output.

Develop a mapping from Maxima help to SAGE help.

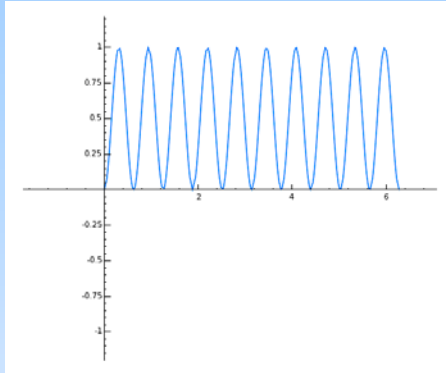
Tool tips to display available member functions\*.

\* I found the tab key...

# Plotting.

```
p1 = plot(lambda x:sin(5*x)^2, 0, 2*pi, rgbcolor=hue(0.6))
```

```
p1.show()
```



```
p2 = plot(lambda x:Real(exp(sqrt(-1)*x)), 0, 2*pi, rgbcolor=hue(0.6))
```

Exception (click to the left for traceback):

...

NameError: global name 'Real' is not defined

## Comments:

- Still working from examples.

```
p1 = plot(lambda x:sin(5*x)^2, 0, 2*pi, rgbcolor=hue(0.6))
```

- How to get it to appear?
- Do you always have to save() first?
- What's lambda?

```
p2 = plot(lambda x:Real(exp(sqrt(-1)*x)), 0, 2*pi, rgbcolor=hue(0.6))
```

- Searchable reference: real, Real, Re, Im?
- Can x be complex?
- Considerable functionality. With some effort (on my part) it might be quite useful as a plotting tool.

## Truncation error analysis.

### Comments:

- Couldn't figure out how to define a "symbolic" function.

$$g := h \rightarrow (f(x+h) - 2*f(x) + f(x-h))/h^2;$$

- Limitations of Maxima or my knowledge of Maxima?

### Possible project targets:

Better organized help? Searchable Reference.

## Why improve usability for the “casual user”.

researcher: “I just want the formula...”

students: “I just want to get my homework done ...”

Too much to ask for?

One has to provide what people expect ...

## As a casual user I rely on “knowledge in the machine”

Why I use Maple: symbolic functionality + a help system that allows me to solve my problems quickly. I forget Maple command constructs.

Why I use Eclipse: IDE functionality + a help system that allows me to quickly remember programming aspects in different languages (Perl, Java, C++). I forget specific language commands/constructs.

Why I use Dreamweaver: Web construction functionality + a help system that allows me to quickly create web pages. I forget web page constructs.

Why I use Scientific Workplace: Tex functionality + a WYSWYG interface to Tex. I forget Tex Constructs.

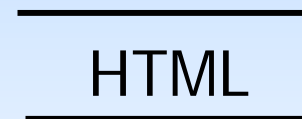
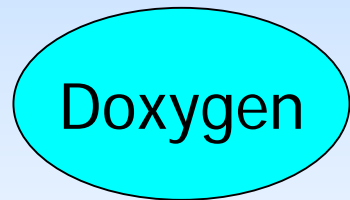
*Why I use SAGE: Symbolic IDE functionality + a help system that allows me to solve my problems quickly. I forget SAGE commands.*

## Experimenting ...

Developing a mapping from Maxima help to SAGE help...

Doxygen?

Header files with  
documentation  
+ samples



This will need some work ...

# Experimenting ...

## CAMsymbolicFunction for creating C code?

Function Input :  $1 - x^2/2 + x^4/12 - x^8/720$

```
//  
// 1 - x^2/2 + x^4/12 - x^8/720  
//  
double evalData[17];  
  
evalData[0] = x;  
evalData[1] = 1;  
evalData[2] = 2;  
evalData[3] = 2;  
evalData[4] = 4;  
evalData[5] = 12;  
evalData[6] = 8;  
evalData[7] = 720;  
evalData[8] = pow(evalData[0],evalData[2]);  
evalData[9] = pow(evalData[0],evalData[4]);  
evalData[10] = pow(evalData[0],evalData[6]);  
evalData[11] = evalData[8] / evalData[2];  
evalData[12] = evalData[9] / evalData[5];  
evalData[13] = evalData[10] / evalData[7];  
evalData[14] = evalData[1] - evalData[11];  
evalData[15] = evalData[14] + evalData[12];  
evalData[16] = evalData[15] - evalData[13];  
return evalData[16];
```



## Summary: An outsider looks at SAGE

### What an outsider sees:

- A tool that could be very useful in “classical” scientific computation work.

The “open source” nature may facility the creation of codes that combine conventional and symbolic computation.

Some work will need to be done to improve ease of use for the casual user.

- A project that’s of interest as a source of problems and collaborations:

Linear algebra\*

High performance computing

...

## Summary: An outsider looks at SAGE

What an outsider sees:

An exciting project. Keep up the good work!