

The Wolfram Language in the HiggsToolset

Eduardo Serna Campillo

Wolfram Technology Group & Algorithm R&D

Wolfram Research, Inc., Champaign, IL, USA

eduardos@wolfram.com

First Annual Meeting of ITN HiggsTools

Albert-Ludwigs Universität Freiburg, Fakultät für Mathematik und Physik

April 15, 2014

Table of Contents

- Wolfram Research
- Mathematica
- *Mathematica* for the particle physicist
- Internship

Wolfram Research

- Wolfram Research was founded by Stephen Wolfram in 1989.
- Heavy bias towards R&D
- Huge user base both in academia and industry
- Present in most universities

Wolfram Technology

- Mathematica
- Wolfram Alpha: knowledge based search engine integrated into Mathematica
- Wolfram Cloud: automated distribution and generation of reports, access *Mathematica* from anywhere
- Wolfram CDF Player: *Mathematica* → generate CDFs → view/interact in Wolfram CDF Player
- ... and many others

A well-established user community



- HEP community prominent member of this community

Extensive support in community webpages

- matematica.stackexchange.com
- <http://community.wolfram.com/>

Mathematica

Front-end

- A powerful IDE
 - Provides code completion
 - Convenient WYSIWG mathematical typesetting
- Every element in the Front end is a Wolfram Language expression: can be programatically manipulated.
- Free-form input: Natural language processing allows one to pick up the language very quickly
- Extensive visualization capabilities

Kernel

- Back-end that performs all the computations.
- Can be dispatched independently and in parallel
- Computations can be monitored remotely (e.g.tablet)

Extensively used in the Physics and Mathematics Communities - I

Symbolic Language

- Fully symbolic language allows us to fully manipulate any expression
 - Can manipulate structurally
- Powerful pattern matcher allows us to match arbitrarily complicated expressions
 - Can manipulate semantically
- Functions in *Mathematica* are defined by rules that act on patterns.
- Very expressive language, Wolfram|Alpha is written in Mathematica
- Built in simplifiers and solvers
- e.g can represent Feynman diagrams and/or arbitrary graphs

Symbolic Computation

- Algebraic Manipulation

`Factor[1 + x + x^2 + x^3]`

$(1 + x) (1 + x^2)$

`Simplify` $\left[\frac{1}{3(1+x)} - \frac{-1+2x}{6(1-x+x^2)} + \frac{2}{3\left(1+\frac{1}{3}(-1+2x)^2\right)} \right]$

$\frac{1}{1+x^3}$

- Solve equations and perform series expansion

`sol = Solve[w^2 - z^3 w + z + z w^5 == 0, w]`

$$\left\{ \left\{ w \rightarrow -i \sqrt{z} \right\}, \left\{ w \rightarrow i \sqrt{z} \right\}, \left\{ w \rightarrow \frac{\left(\frac{2}{3}\right)^{1/3} z^2}{\left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}} + \frac{\left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}}{2^{1/3} 3^{2/3} z} \right\} \right\},$$

$$\left\{ w \rightarrow -\frac{\left(1 + i \sqrt{3}\right) z^2}{2^{2/3} 3^{1/3} \left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}} - \frac{\left(1 - i \sqrt{3}\right) \left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}}{2 \times 2^{1/3} 3^{2/3} z} \right\},$$

$$\left\{ w \rightarrow -\frac{\left(1 - i \sqrt{3}\right) z^2}{2^{2/3} 3^{1/3} \left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}} - \frac{\left(1 + i \sqrt{3}\right) \left(-9 z^2 + \sqrt{3} \sqrt{27 z^4 - 4 z^9}\right)^{1/3}}{2 \times 2^{1/3} 3^{2/3} z} \right\}$$

`Series[w /. sol[[3]], {z, 0, 5}]`

$-\frac{(-1)^{2/3}}{z^{1/3}} + \frac{1}{3} (-1)^{1/3} z^{4/3} + \frac{1}{81} (-1)^{2/3} z^{14/3} + O[z]^{16/3}$

- Calculus

■ Integration and Differentiation

$$\int_{-\infty}^{\infty} (1 + x^2 + x^6) e^{-x^2} dx$$

$$\frac{27\sqrt{\pi}}{8}$$

$$D\left[\frac{x^2 + 3x - 2}{x^5 + 6x^2 + 1}, \{x, 2\}\right]$$

$$-\frac{2(3+2x)(12x+5x^4)}{(1+6x^2+x^5)^2} + \frac{2}{1+6x^2+x^5} + (-2+3x+x^2) \left(\frac{2(12x+5x^4)^2}{(1+6x^2+x^5)^3} - \frac{12+20x^3}{(1+6x^2+x^5)^2} \right)$$

■ Differential Equation

$$\text{eqs} = \{x'[t] == v[t], v'[t] == \frac{-1}{2} v[t] - x[t], x[0] == 1, v[0] == 0\};$$

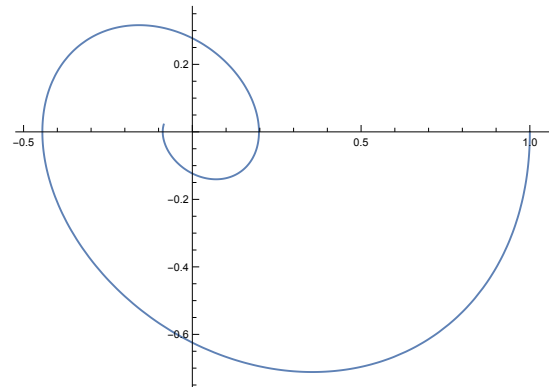
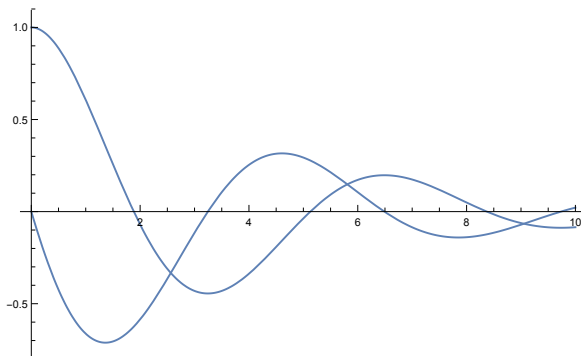
`sol = DSolve[eqs, {x, v}, t]`

$$\left\{ \left\{ v \rightarrow \text{Function}[t], -\frac{4 e^{-t/4} \sin\left[\frac{\sqrt{15} t}{4}\right]}{\sqrt{15}} \right\}, \right.$$

$$\left. x \rightarrow \text{Function}[t], \frac{1}{15} e^{-t/4} \left(15 \cos\left[\frac{\sqrt{15} t}{4}\right] + \sqrt{15} \sin\left[\frac{\sqrt{15} t}{4}\right] \right) \right\}$$

`GraphicsRow[{Plot[{x[t], v[t]} /. sol, {t, 0, 10}],`

`ParametricPlot[{x[t], v[t]} /. sol, {t, 0, 10}], ImageSize -> 1000]`



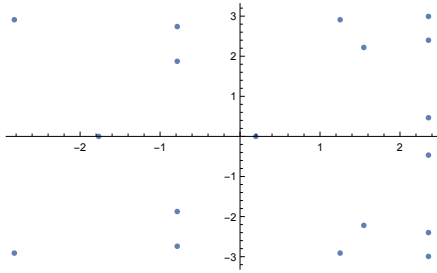
Numerical Computation

■ Solve nonlinear equations numerically

`roots = NSolve[{Sin[z + Sin[z]] == Cos[z + Cos[z]], -3 < Re[z] < 3, -3 < Im[z] < 3}, z]`

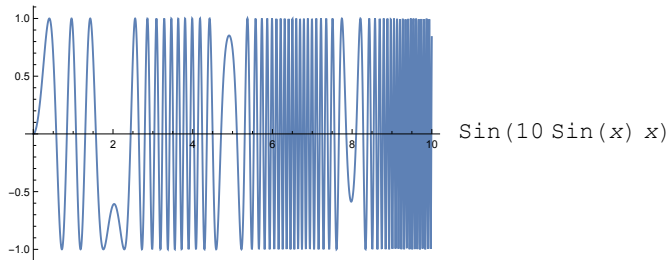
```
{z -> -2.82249 - 2.91043 i}, {z -> -2.82249 + 2.91043 i}, {z -> -1.76794},
{z -> -0.785398 - 1.87345 i}, {z -> -0.785398 + 1.87345 i}, {z -> -0.785398 - 2.7399 i},
{z -> -0.785398 + 2.7399 i}, {z -> 0.197147}, {z -> 1.2517 - 2.91043 i}, {z -> 1.2517 + 2.91043 i},
{z -> 1.54771 - 2.21877 i}, {z -> 1.54771 + 2.21877 i}, {z -> 2.35619 - 0.466339 i},
{z -> 2.35619 + 0.466339 i}, {z -> 2.35619 - 2.39939 i}, {z -> 2.35619 + 2.39939 i},
{z -> 2.35619 - 2.99287 i}, {z -> 2.35619 + 2.99287 i}
```

`ListPlot[Transpose[{Re[#], Im[#]}] &[z /. roots]`



■ Numerical Integration

```
Plot[Sin[10 Sin[x] x], {x, 0, 10}, PlotRange -> All, PlotLegends -> "Sin(10 Sin(x) x)"]
```



```
Print[# -> AbsoluteTiming@
```

```

  NIntegrate[Sin[10 Sin[x] x], {x, 0, 10}, Method -> {"LocalAdaptive", Method -> #}] & /@
  {"RiemannRule", "NewtonCotesRule", "TrapezoidalRule", "ClenshawCurtisRule",
   "GaussKronrodRule", "LevinRule", "LobattoKronrodRule"};
RiemannRule -> {1.79334, -0.158815}
NewtonCotesRule -> {0.0321796, -0.159716}
TrapezoidalRule -> {0.0407915, -0.159716}
ClenshawCurtisRule -> {0.00961733, -0.159716}
GaussKronrodRule -> {0.0105374, -0.159716}
NIntegrate::nonlev: Integrand Sin[10 x Sin[x]] is not a Levin function. >>
NIntegrate::mtdfb: Numerical integration with LevinRule failed. The integration continues with Method -> GaussKronrodRule. >>
LevinRule -> {0.237713, -0.18745}
LobattoKronrodRule -> {0.00724938, -0.159716}

```

■ NDSolve

KdV equation: $u_t + u_{xxx} + 3(u^2)_x = 0$

```
eq = D[u[x, t], t] + D[u[x, t], {x, 3}] + 3 D[u[x, t]^2, x] == 0;
```

```
pbcs = {u[-15, t] == u[15, t], u(1,0)[-15, t] == u(1,0)[15, t], u(2,0)[-15, t] == u(2,0)[15, t]};
```

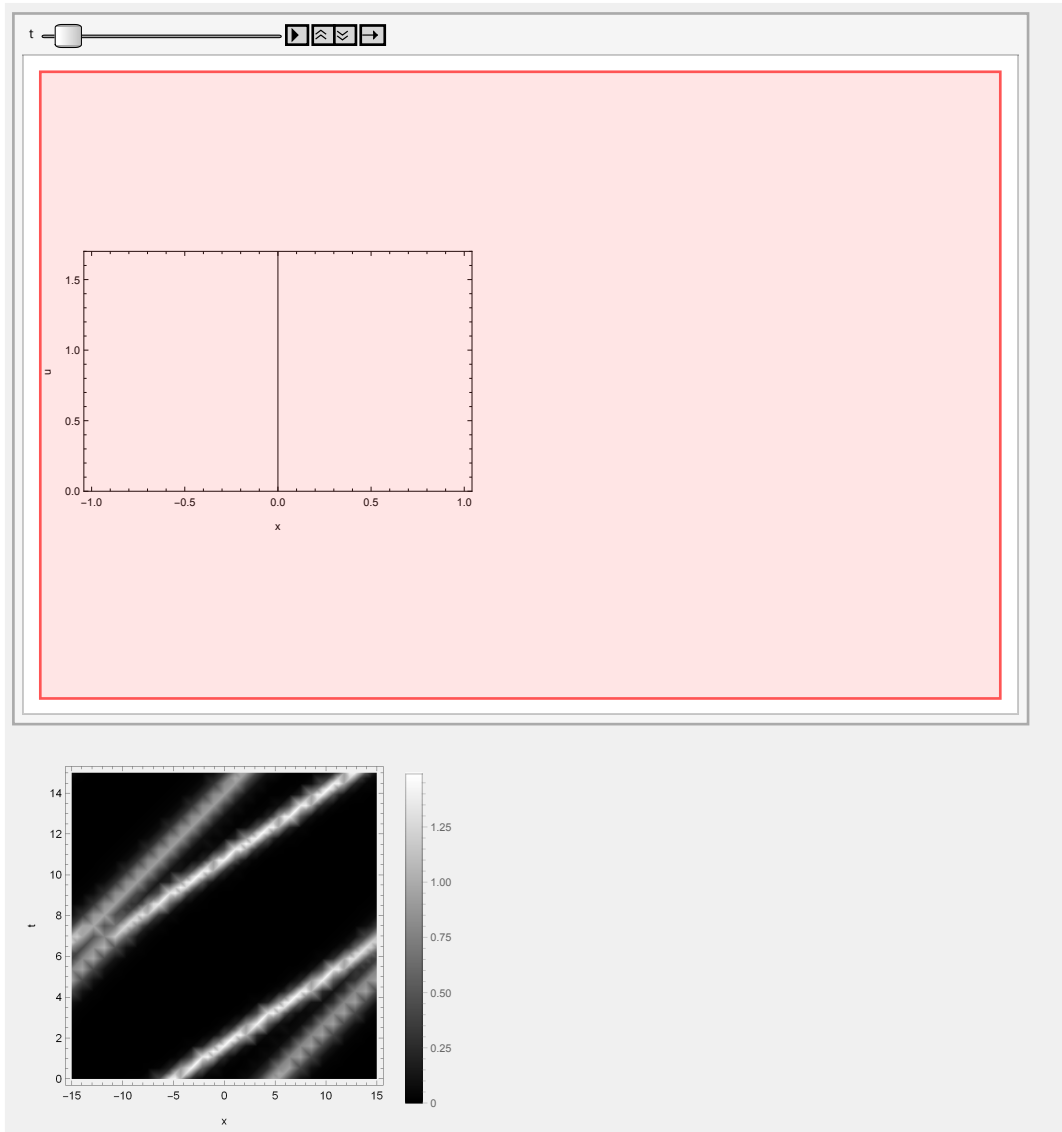
```
ics = u[x, 0] == 0.5 (2 Sech[0.5 Sqrt[2] (x - 5)]^2 + 3 Sech[0.5 Sqrt[3] (x + 5)]^2);
```

```
usol =
```

```

  Quiet@NDSolve[{eq, pbcs, ics}, u, {x, -15, 15}, {t, 0, 15}, Method -> "StiffnessSwitching"];
Panel[Row[{Animate[Plot[u[x, t] /. usol[[1]], {x, -15, 15},
  PlotRange -> {0, 1.7}, PlotStyle -> Black, Frame -> True, FrameLabel -> {"x", "u"},
  {t, 0, 15}, TrackedSymbols -> t, AnimationRunning -> False], Spacer[30],
  DensityPlot[u[x, t] /. usol[[1]], {x, -15, 15}, {t, 0, 15}, ColorFunction -> GrayLevel,
  ImageSize -> {300, 300}, FrameLabel -> {"x", "t"}, PlotLegends -> Automatic]},
  Alignment -> {Center, Center}], Appearance -> "Frameless"]

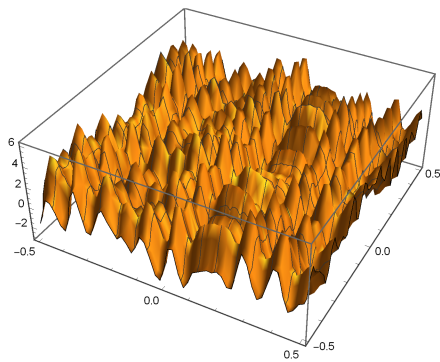
```



■ Numerical Optimization

Search for global minimum with a set of random initial positions

$$f(x, y) = e^{\sin(50x)} + \frac{1}{4}(x^2 + y^2) + \sin(60e^y) - \sin(10(x+y)) + \sin(70 \sin x) + \sin(\sin(80y))$$



```

NMinimize[eSin[50 x] +  $\frac{1}{4}$  (x2 + y2) + Sin[60 ey] - Sin[10 (x + y)] + Sin[70 Sin[x]] + Sin[Sin[80 y]],
{x, y}, Method -> {"RandomSearch", "SearchPoints" -> 100}]
{-3.14408, {x -> -0.0231678, y -> -0.494213}}

```

Units Framework

```
DSolve[{x'[t] == 5 m/s}, x[t], t]
```

```
{{x[t] -> C[1] + (5 m/s) t}}
```

```
DSolveValue[{x''[t] == 5 m/s2, x[0 s] == 3 m, x'[0 s] == 7 m/s}, x[t], t]
```

```
3 m + (7 m/s) t +  $\left(\frac{5}{2} \text{ m/s}^2\right) t^2$ 
```

```
Integrate[x, {x, Quantity[0, "Meter"], Quantity[1, "Meter"]}]
```

```
 $\frac{1}{2} \text{ m}^2$ 
```

- Support for Natural Units coming soon

Extensively used in the Physics and Mathematics Communities - II

Platform for many tools relevant to particle physics

- FeynRules
- FeynCalc
- FeynArts
- FormLink
- Sigma + others from RISC
- FormCalc
- Package-X
- LOOL
- xTras
- ... and many others

Visualization

Function visualization	Data visualization	Business charting	Special visualization	Graph visualization

Save As ► L^AT_EX

`BesselI[2, 3] // TeXForm`

`I_2(3)`

Extensive Import-Export capabilities

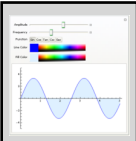
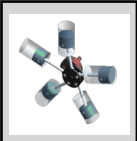
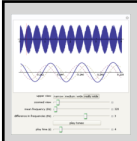
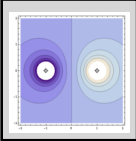
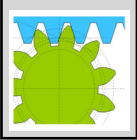
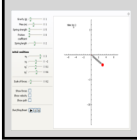

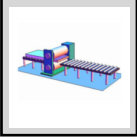
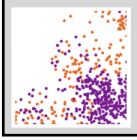
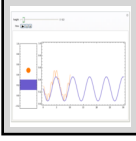
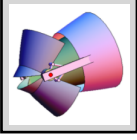
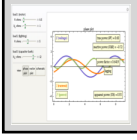
Basic formats | Multimedia | Data | Specialized areas | Documents | Other

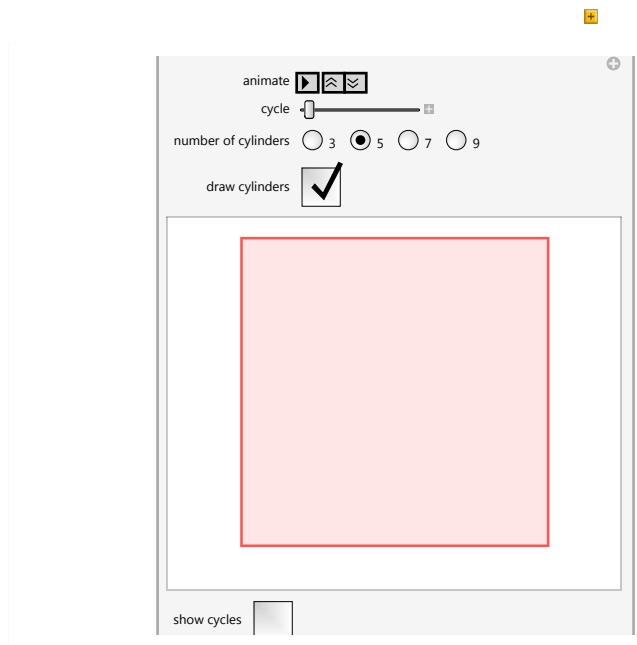
Tabular & Spreadsheet Formats
{Table, CSV, TSV, XLS, ODS, SXS, ...}

Database Formats
{MDB, DBF, DIF, XLS, ...}

- e.g. HDF5

Dynamic Interactivity

Everyday Tasks	Modeling	Simulations
		
		
		
		

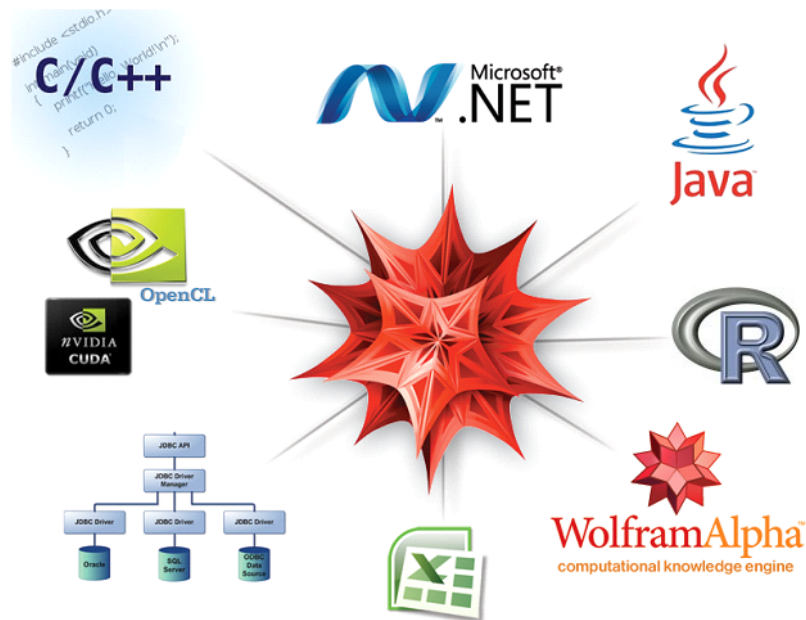


The screenshot shows a software interface for a simulation. At the top right, there is a small yellow square icon. Below it, the interface has a control panel with the following elements:

- animate**: A play button icon.
- cycle**: A slider control.
- number of cylinders**: Four radio buttons labeled 3, 5, 7, and 9. The button for 5 is selected.
- draw cylinders**: A checked checkbox.

The main area of the interface is a large white rectangle with a red border, which is currently empty. At the bottom left of this area, there is a **show cycles** checkbox, which is currently unchecked.

Connecting *Mathematica* to other programs / languages



LibraryLink

- Integrate external dynamic linked libraries (DLLs) into *Mathematica* for high-speed, memory-efficient execution.

DataBaseLink

- SLAM, a *Mathematica* interface for SUSY spectrum generators
- “...automatic saving and loading of SUSY spectra to and from a SQL data base, avoiding the rerun of a spectrum generator for a known spectrum”

Performance:

- Vectorised implementations use efficient Machine and Extended Precision
- Easy access to Paralellization
- Ability to Compile
- We can optimize the looping construct by using Compile.

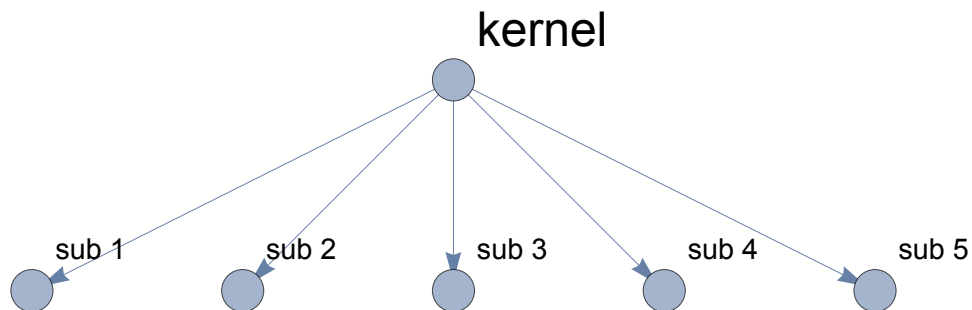
```
{procedural2, procedural3} = Compile[{{list, _Real, 1}}, Block[
  {max = -2., maxdrawdown = 0., temp},
  Do[If[(temp = list[[n]]) > max, max = temp,
    If[max - temp > maxdrawdown, maxdrawdown = max - temp]], {n, Length[list]};
  maxdrawdown], CompilationTarget -> #] & /@ {"WVM", "C"};
AbsoluteTiming@procedural2[proc]
AbsoluteTiming@procedural3[proc]
```

Parallel Computing

Vectorization

Automated Parallelization

Kernel based parallelization

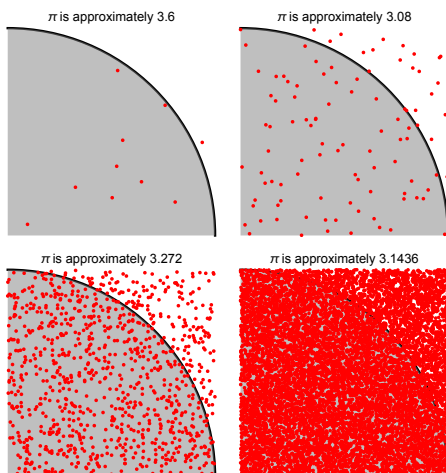


1. Communication is always controlled through the controlling kernel
2. Parallelization is automated through the use of Parallelize (and related functions)
3. Lower level parallel operations can be handled through ParallelSubmit and ParallelEvaluate

■ Local subkernels

LaunchKernels[]

Using ParallelEvaluate to easily parallelize a Monte-Carlo method



```

f[n_Integer] := 4.0 Count[RandomReal[{0, 1}, {n, 2}], xy_ /; Norm[xy] < 1] / n
DistributeDefinitions[f]
Mean[With[{n = 10^6}, ParallelEvaluate[f[n]]]] // AbsoluteTiming
  
```

```
With[{n = 10^6}, f[4 n]] // AbsoluteTiming
CloseKernels[]
```

- Manual remote subkernels

Using remote shell invocation technology

<http://stackoverflow.com/questions/6783840/how-to-configure-parallel-remote-kernels-in-mathematica>

- Lightweight Grid Manager

- Cluster Integration Tools

GPU computing

- OpenCLLink

- CUDALink

```
Needs["CUDALink`"]
CUDAQ[]
```

CUDADot

```
CUDADot[N@Table[i, {i, 10}, {j, 10}], N@Table[i, {i, 10}, {j, 10}]] // MatrixForm
```

CUDAFold

```
Fold[f, x, Range[5]]
CUDAFold[Plus, 0, Range[10 000 000]] // AbsoluteTiming
Fold[Plus, 0, Range[10 000 000]] // AbsoluteTiming
```

Internship Program - I

- Three+ month internships in Champaign Headquarters
- Opportunity to hone *Mathematica* skills by choosing from a range of supervised projects
- *Mathematica* experience useful but training from scratch available
- Great opportunity to see life on the other side of the fence
- Great career building opportunity
- Interview: CV, code examples and a chat
- Batches of 2-3, team up for housing, learning and keeping each other warm

Internship Program - II

- I was an intern a year ago with LHCPHENONET, HIGGSTOOLS predecessor
- My previous *Mathematica* experience allowed me to jump into a project straight away
- Worked on two projects:
 - Efficient calculation of sequences defined by recurrence relations
 - Use of graph theory algorithms for separation of statistically independent subexpressions
- The experience was very fun for me, relevant algorithms span many different areas of Mathematics, I learnt an incredible amount
- Broader, less specialized learning compared to PhD

Internship Program - III

- Champaign is a nice university town
- One of the best public universities in the world, intellectual atmosphere in town
- Chicago is doable in the weekends

```
GeoGraphics@GeoPath[{Champaign (city), Chicago (city)}]
```

```
GeoDistance[Champaign (city), Chicago (city), UnitSystem -> "Metric"]
```

- Housing is provided by Wolfram, but only if they have some available
- Avoid freezing winter (January, February)
- Technology Conference in October is a good time to come

Conclusion

- Wolfram is company with a long history of R&D in the cutting edge
- Huge user base both in academia and industry
- Symbolic language gives lots of flexibility and speed of implementation
- HEP community has built sophisticated tools on top of Mathematica
- Fully integrated, high quality multi-domain visualizations
- Easy connectivity to more specialised tools, e.g. FORM
- Easy access to parallelization
- Internships are a valuable and fun opportunity

Thank you for your attention !

⋮