COMPUTATIONAL ASPECTS OF PAIR PRODUCTION FROM STRONG FIELDS

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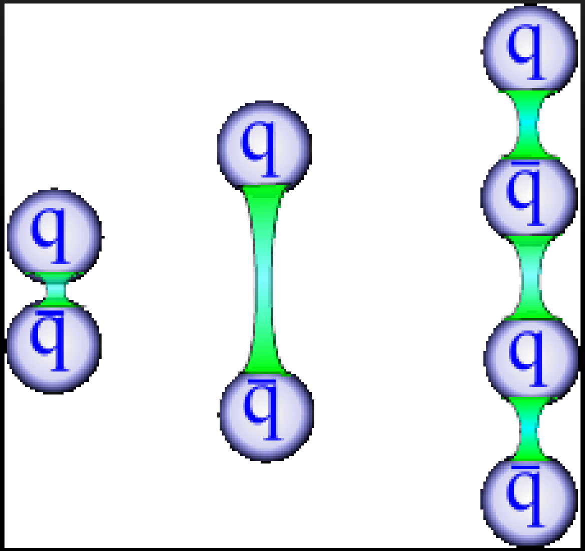
MOTIVATION

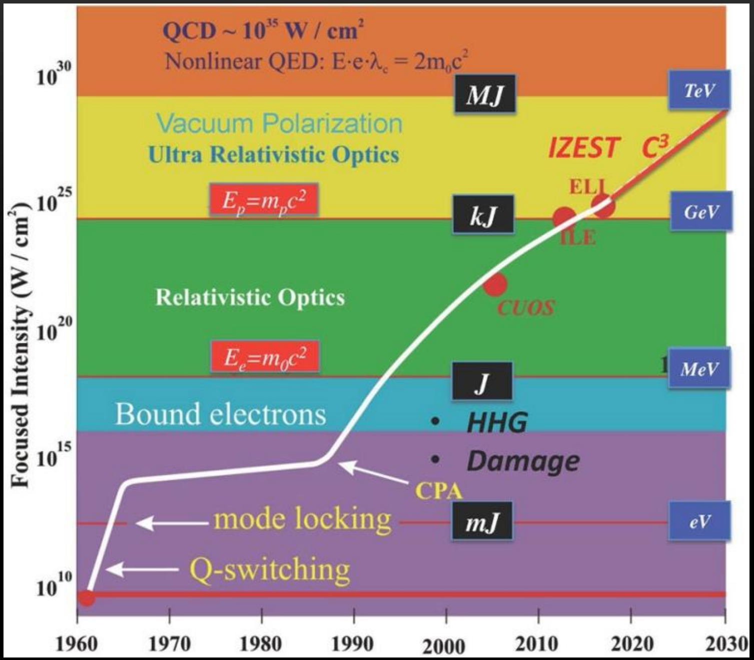
- Pair production from vacuum:
  - $q\bar{q}$ in heavy ion collisions:
    - Description of the early stages of collisions,
    - Formation and breaking of color strings,
    - Successful family of models,
    - Understanding of LHC data, particle spectras, etc.



MOTIVATION

- Pair production from vacuum:
  - e^+e^- in extreme strong laser fields:
    - Holy grail of QED
    - interesting non-linear phenomena in this regime

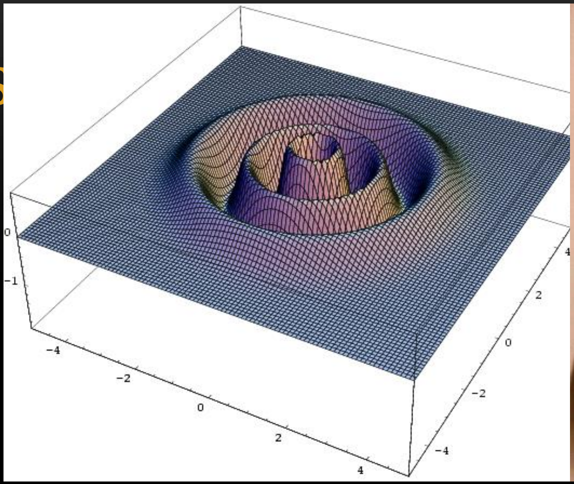
  - Also possible near compact astrophysical objects



T. Tajima, G. Mourou

THEORETICAL MODEL

- We use Wigner-functions to model pair production
- Quantum analogue of the classical one particle distribution function



Eugene Wigner

- Definition:

$$\hat{C}\,(\vec{x},\vec{s},t) = \exp\left(-iq\int_{-1/2}^{1/2}\vec{\boldsymbol{A}}(\vec{x}+\lambda\vec{s},t)\vec{s}\,\mathrm{d}\lambda\right)\left[\Psi\left(\vec{x}+\frac{\vec{s}}{2}\right),\bar{\Psi}\left(\vec{x}-\frac{\vec{s}}{2}\right)\right]$$

$$\boldsymbol{W}(\vec{\boldsymbol{x}},\vec{\boldsymbol{p}},\boldsymbol{t}) = -\frac{1}{2}\int e^{-i\vec{p}\vec{s}}\left\langle 0\middle|\hat{C}\,(\vec{x},\vec{s},t)\middle|0\right\rangle \mathrm{d}\vec{s}$$

I. Bialynicki-Birula et al, Phys. Rev. **D44**, 1825-1835. (1991)

THEORETICAL MODEL

- Hartee-type approximation: $\langle F^{\mu\nu} C \rangle \to \langle F^{\mu\nu} \rangle \langle C \rangle$
- No back reaction, no radiation corrections, etc.
- Compact form of evolution equation:

$$\boldsymbol{D_t W} = -\frac{1}{2}\overrightarrow{\boldsymbol{D}}_{\vec{x}}[\gamma^0\vec{\gamma}, \boldsymbol{W}] - im[\gamma^0, \boldsymbol{W}] - i\overrightarrow{\boldsymbol{P}}\{\gamma^0\vec{\gamma}, \boldsymbol{W}\}$$

- The differential operators are non trivial operator series:

$$\boldsymbol{D_t} = \partial_t + e\overrightarrow{\boldsymbol{E}}\vec{\nabla}_p + \ldots$$

- Expansion on 4x4 Dirac basis:

$$\boldsymbol{W}(x, p, t) = \frac{1}{4}\left[1\mathbb{s} + i\gamma_5\mathbb{p} + \gamma^\mu\mathbb{v}_\mu + \gamma^\mu\gamma_5\mathbb{a}_\mu + \sigma^{\mu\nu}\mathbb{t}_{\mu\nu}\right]$$

THEORETICAL MODEL

- Time evolution equations:

  A Boltzmann like equations for the quantum one particle distribution function:
  (QED: 3+3+1 dimension, 16 components, F. Hebenstreit et al, Phys. Rev. **D82** (2010) 105026.)

$$\begin{array}{lllllll}
D_t\mathbb{s} & & & - & 2\vec{P}\cdot\vec{\mathbb{t}}_1 & = 0 \\
D_t\mathbb{p} & & & + & 2\vec{P}\cdot\vec{\mathbb{t}}_2 & = 2m\mathbb{a}_0 \\
D_t\mathbb{v}_0 & + & \vec{D}_{\vec{x}}\cdot\vec{\mathbb{v}} & & & = 0 \\
D_t\mathbb{a}_0 & + & \vec{D}_{\vec{x}}\cdot\vec{\mathbb{a}} & & & = 2m\mathbb{p} \\
D_t\vec{\mathbb{v}} & + & \vec{D}_{\vec{x}}\mathbb{v}_0 & + & 2\vec{P}\times\vec{\mathbb{a}} & = -2m\vec{\mathbb{t}}_1 \\
D_t\vec{\mathbb{a}} & + & \vec{D}_{\vec{x}}\mathbb{a}_0 & + & 2\vec{P}\times\vec{\mathbb{v}} & = 0 \\
D_t\vec{\mathbb{t}}_1 & + & \vec{D}_{\vec{x}}\times\vec{\mathbb{t}}_2 & + & 2\vec{P}\mathbb{s} & = 2m\vec{\mathbb{v}} \\
D_t\vec{\mathbb{t}}_2 & - & \vec{D}_{\vec{x}}\times\vec{\mathbb{t}}_1 & - & 2\vec{P}\mathbb{p} & = 0
\end{array}$$

THEORETICAL MODEL

- In case of no magnetic field (B=0) and homogeneous electric field (E(t)):

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{dt}} = \frac{\mathrm{eE}\varepsilon_{\perp}}{\omega^2}\mathrm{v}$$

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{dt}} = \frac{1}{2}\frac{eE\varepsilon_{\perp}}{\omega^2}(1-2f)-2\omega u$$

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = 2\omega u$$

where:

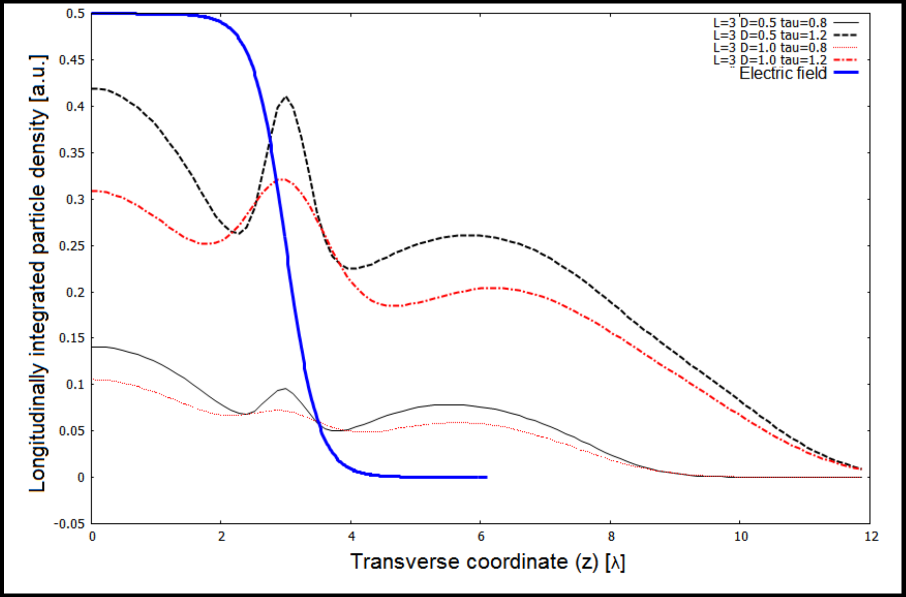
$$\vec{p} = \left(\vec{q}_{\perp}, q_{\parallel} - eA(t)\right)$$

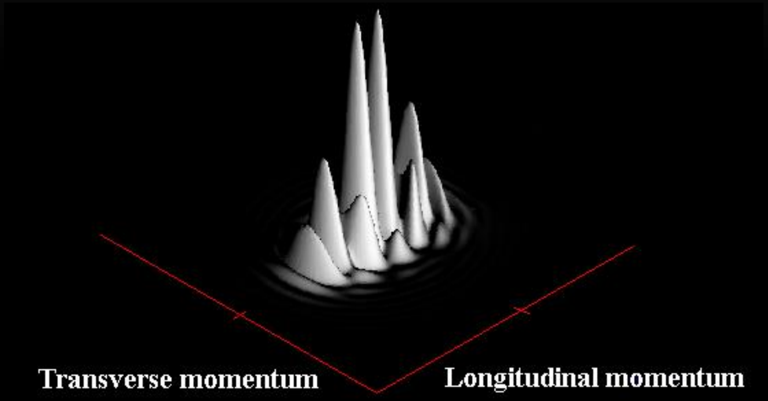
THEORETICAL MODEL

- The Wigner function based description can be extended to higher symmetries (non-Abelian case) too.
  (Quark Wigner function evolution: A.V. Prozorkevich, S.A. Smolyansky, S.V. Ilyin)
- There will be more and more components
- The intermixing of components will be more complex (cannot be reduced to an ODE!)
- If the SU(N) color matrices replaced by unity, the QED equations are recovered.

PHYSICS

- We can calculate asymptotic ($t \to \infty$) Wigner functions, so we have:
- Energy-, Momentum-, Mass-, Charge- and Spindensity.
- We can calculate particle spectras:





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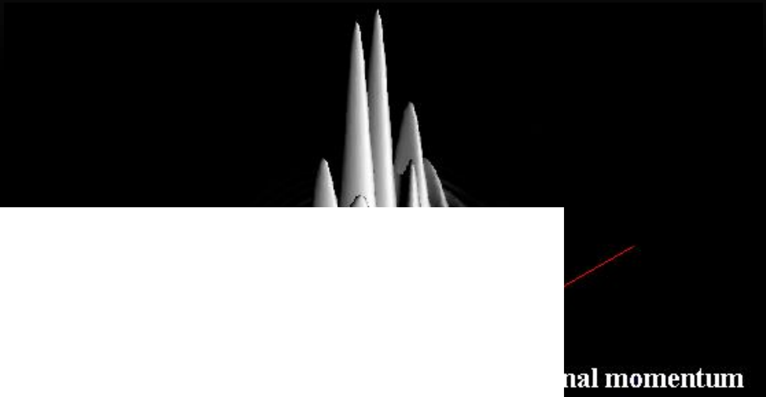

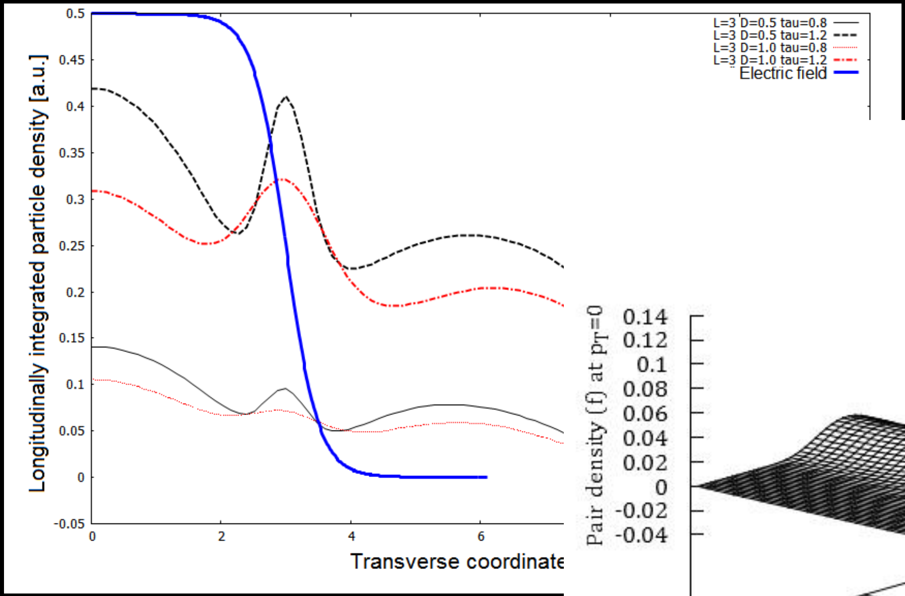

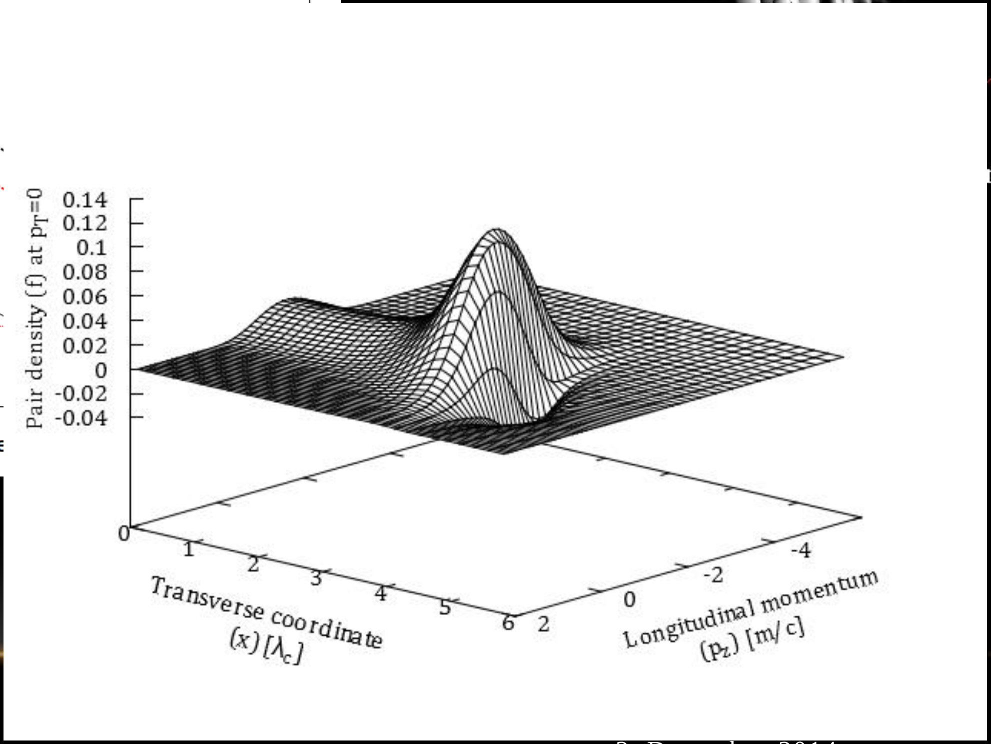

COMPUTATIONAL ASPECTS

Challenges of the evolution equations:

- Too many dimensions $\rightarrow$Simplified configurations are obligatory
  Magnetic field usually neglected
- Handling of the non-local differential operators is not trivial
- Extreme separation of time scales for realistic field parameters
- But most importantly:
  extremely intense computational problem!

LOCAL PROGRAMMING ASPECTS

- One may choose among **many numerical solver methods.**
- The final equations are dependent on the **electromagnetic vector field** configuration addressed.
- **One may not want to rewrite completely the equations each time, when the functional dependence**, especially when some components chosen to be or turn out to be zero…

- More automatization is welcome. Same for (language, API) portability!
- In many cases development resources are more constrained than hardware resources!
- Can we use one tool and less development time**?**
- Can't we generate the final code**?** Possibly from the symbolic equations**?**

PROGRAMMING ASPECTS

If you have an extreme computational problem you will be sent to a super computing center… BUT!

Diversifying parallel architectures: hybrid clusters (**GPUs**), cloud, etc…

You probably don't want to delve into GPU programming…

Nor want to know about the uncountable competing APIs…

BUT!
If your code does not utilize hardware properly, your application for computing time will be

rejected!

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BUT!

If your code does not utilize hardware properly, your application for computing time will be

rejected!

How long will your code maintain its performance?

PROPOSED SOLUTION

- Run-time construction and manipulation of the expression tree from the symbolic equations and dynamic code-generation!

- So:
  - we can support many language back-ends and APIs
  - infer as much as possible from the symbolic equations!
  - eliminate many error sources and inconsistencies!

PROPOSED SOLUTION

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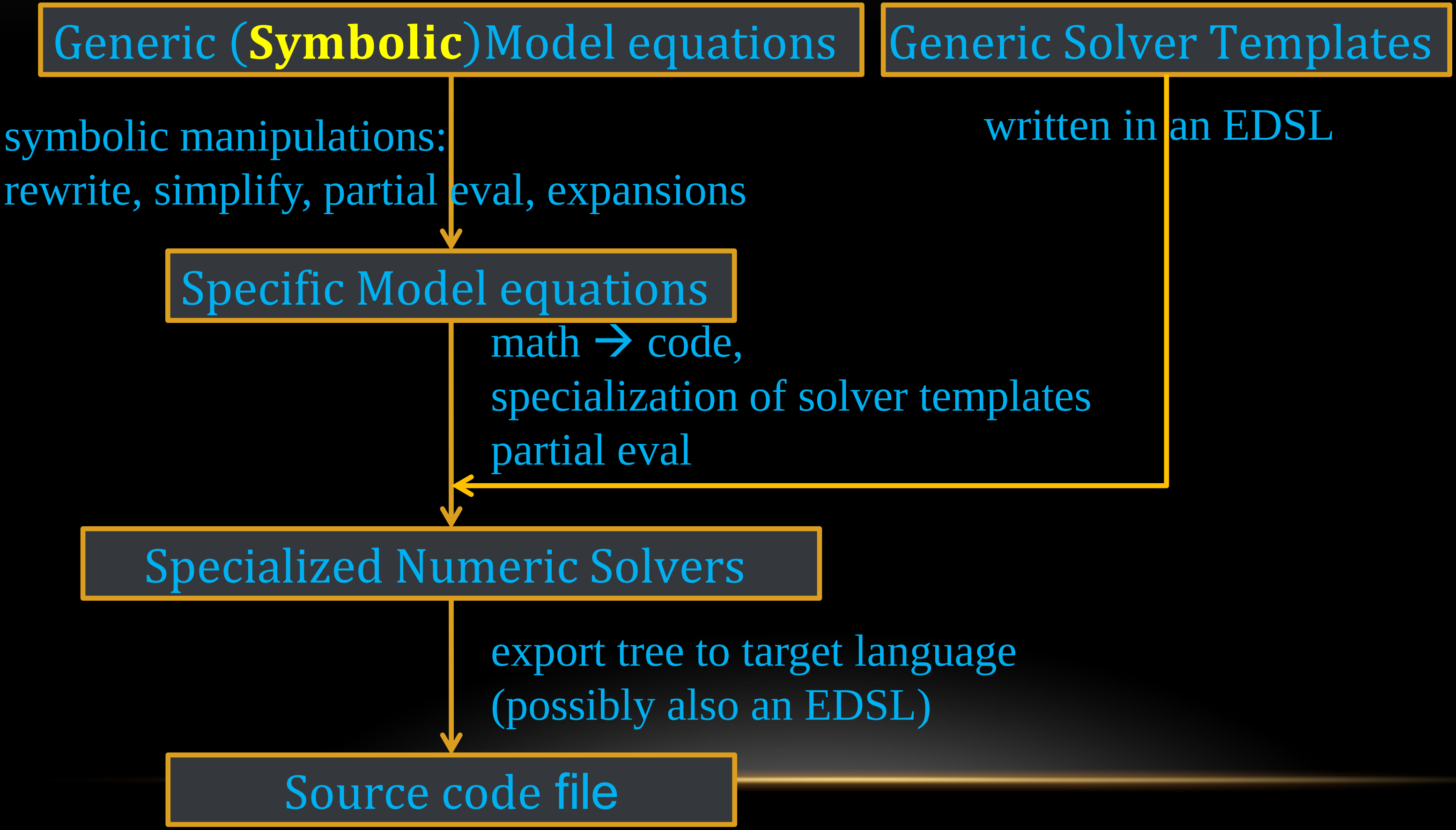
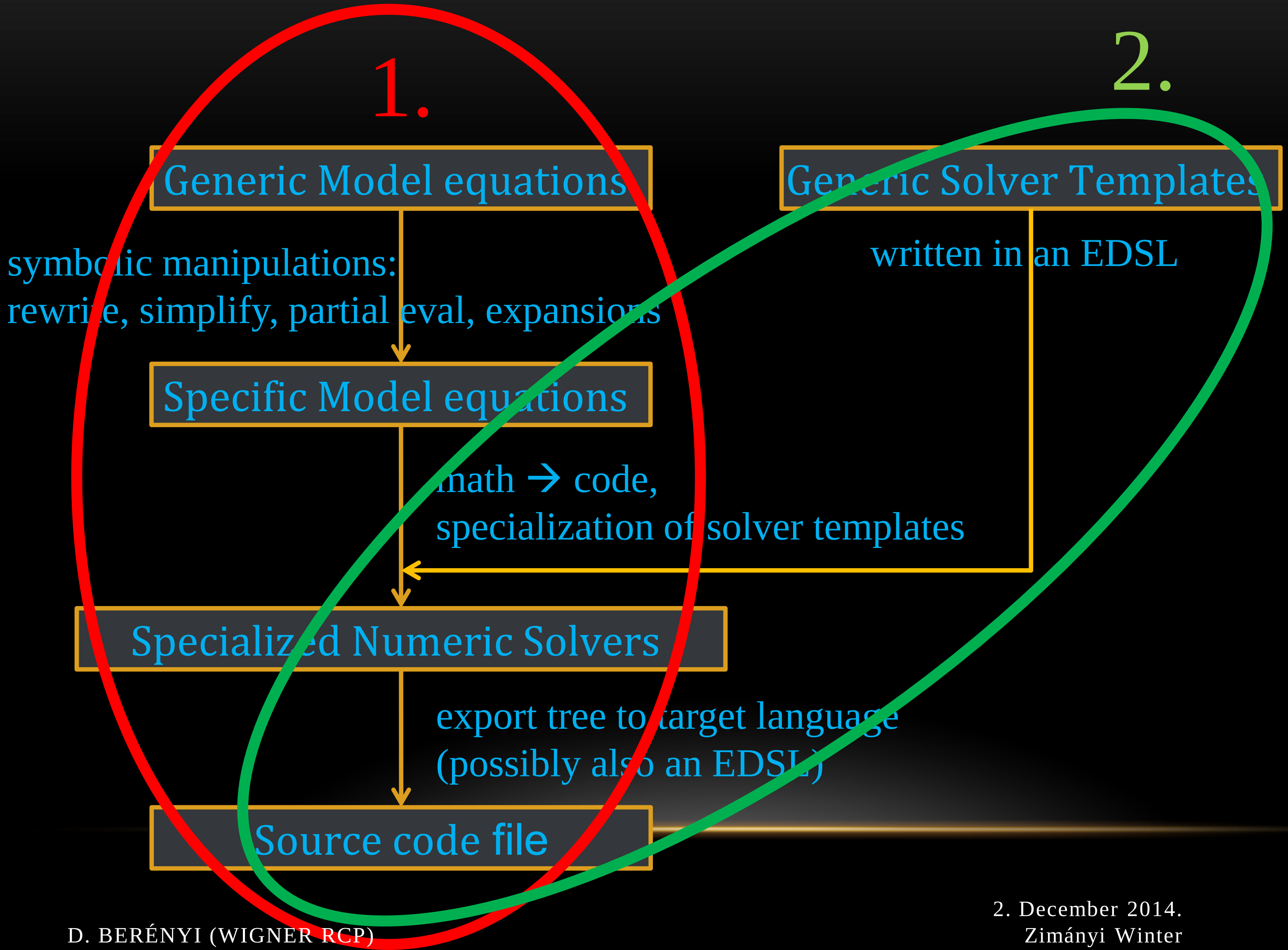
- So:
  - we can support many language back-ends and APIs
  - infer as much as possible from the symbolic equations!
  - ~~eliminate~~ many error sources and inconsistencies!

exterminate

CODE-GENERATION FLOW


Generic (**Symbolic**)Model equations
Generic Solver Templates
symbolic manipulations:
rewrite, simplify, partial eval, expansions
written in an EDSL
Specific Model equations
math → code,
specialization of solver templates
partial eval
Specialized Numeric Solvers
export tree to target language
(possibly also an EDSL)
Source code file

CODE-GENERATION FLOW



CURRENT STATUS

- In the case of a homogeneous electric field, the equation system is a 3 component ODE, it decouples in the momentum variable.

- In this case the 2. method was fully implemented (parallelized over the momentum variable).

- The resulting speed-up is around 30x

- The symbolic part of the PDE solver in the 1. method was successfully tested on simple equations:
  Fokker-Planck/Differential Vlasov equation

SUMMARY

- Pair production is an interesting high energy phenomena with applications in QCD as well as in QED!

- However the modeling is computationally demanding and requires novel development tools.

Code generation from Abstract Syntax Trees is a nice versatile tool because:

- Can represent constructs from Mathematics and Programing and easily map to source code
- Symbolic manipulations can be performed
- Reusable, flexible language independent solver templates can be created
- Can generate all the low-level buffer manipulation between the CPU and GPU.

High-performance user friendly differential equation solvers are almost here!

This work was supported by the Hungarian OTKA Grants No. 104260, No. 106119.

THANK YOU

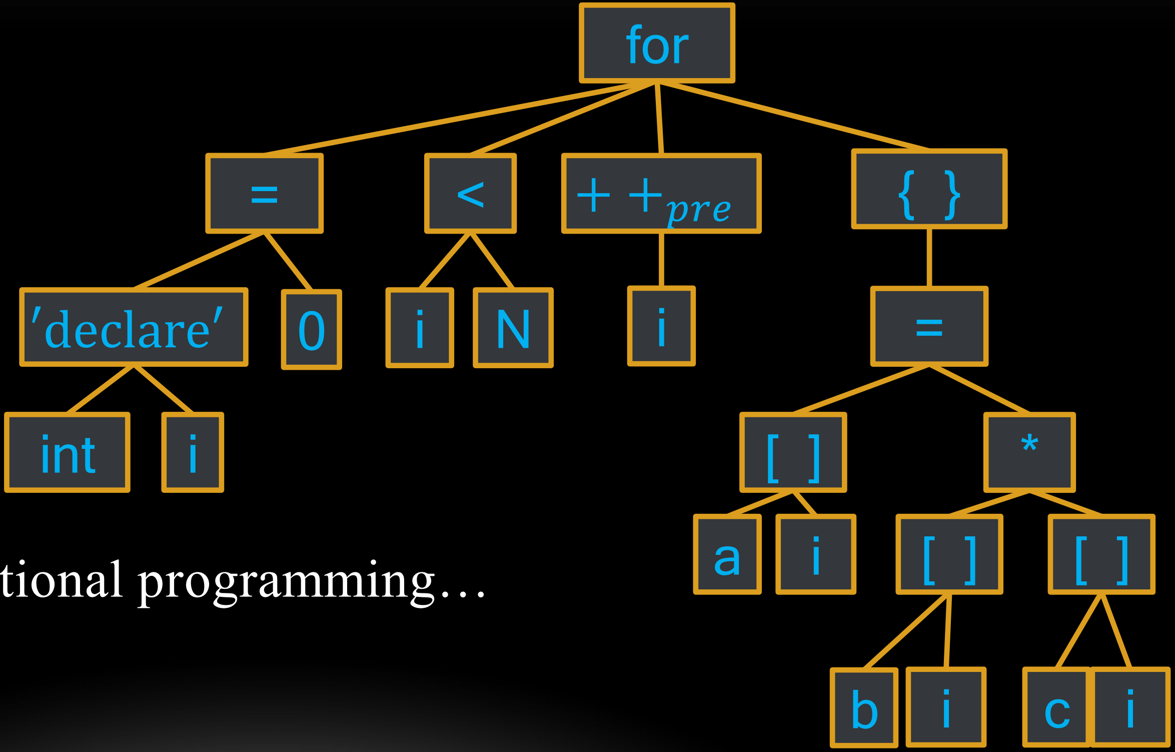
- Questions?

BACKUP SLIDES

ABSTRACT SYNTAX TREES

- Imperative programming constructs can also be represented by trees:

```
for(int i=0; i<N; ++i)
{
    a[i] = b[i] * c[i];
}
```



- Not to mention functional programming…

WORKFLOW

- The expected workflow is:

1. Formulation
   (mathematical equations, symbolic manipulation)

2. Spectral expansion into a dense matrix problem
   (maybe inside a finite difference time integrator)

3. Efficient parallel implementation/execution

- Possible tools:

1. Maxima, Mathematica, …

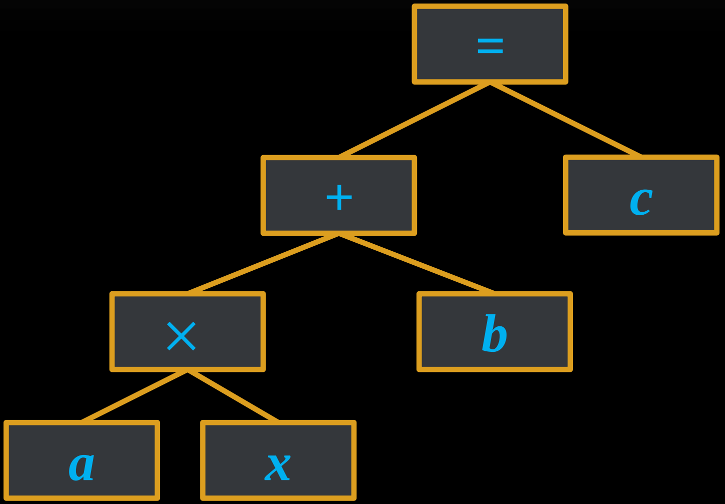
2. Maxima, Mathematica, …
   with or exported to
   Host high level language: C++, Fortran…

3. Parallel APIs & libraries:
   OpenCL, CUDA, …
   BLAS implementations…

ABSTRACT SYNTAX TREES

- Mathematical formulas and equations can be represented by trees:

$$ax + b = c$$



AST MANIPULATIONS

Since all of the needed constructs are trees the workflow can be seen as a series of transformations on the ASTs!

- Symbolic (math) stage:

  simplifications ($0 \cdot a \to a$, $3a + 4a \to 7a$)

  symbolic differentiation ($\frac{d\sin(x)}{dx} \to \cos(x)$)

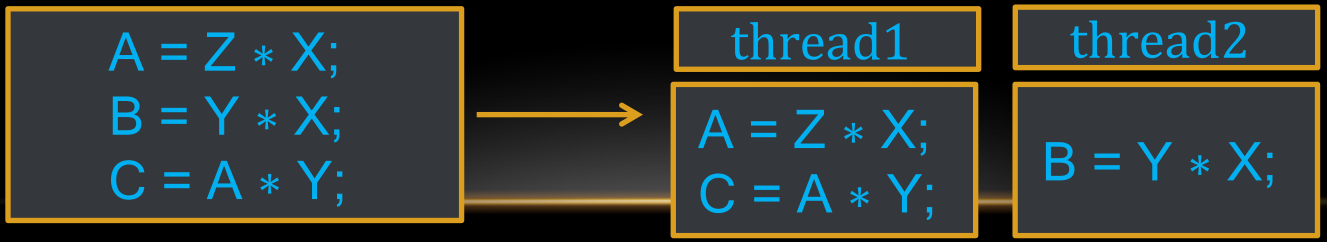
  series expansions ($f(x) \to \sum_{i=0}^{n} f_i \Phi_i\,(x)$)
  check for argument sanity and rank mismatch

- Programming stage:

  Infer types, further sanity checks

a = dot(vector<2, double>(2., 9.) , vector<2, double>(1., 0.)) →a is scalar double

Parallelization from data dependency (consider matrix operations):



```
A = Z * X;
B = Y * X;
C = A * Y;
```

```
A = Z * X;
C = A * Y;
```

```
B = Y * X;
```

AST MANIPULATIONS

At the symbolic stage a general model is specialized according to user defined constants and parameters and simplified symbolically. Numerical solvers are just higher-order functions operating on the equations.

Example: Spectral Expansion (like Fourier, Chebyshev series)

1. Equation:

$$\boxed{\frac{df(x)}{dx} = -af(x)}$$

2. Expansion: $f(x) = \sum_{i=0}^{N} f_i \Phi_i(x)$

$$\boxed{\sum_{i=0}^{N} f_i \frac{d\Phi_i(x)}{dx} = -a \sum_{i=0}^{N} f_i \Phi_i(x)}$$

3. Differentiation: $\Phi_i(x) = \cos(iNx)$

$$\boxed{-\sum_{i=0}^{N} f_i iN\sin(iNx) = -a \sum_{i=0}^{N} f_i \cos(iNx)}$$

SYMBOLIC→PROGRAMMING CONVERSION

All Math objects are given a type deduced from the leaves and propagated upwards.

Function definitions, signatures constructed, defunctionalization applied.

One important construct: ParallelFunction created from vector, matrix operations!

$$f1(a, \vec{x}, \vec{y}) := a\vec{x} + \vec{y}$$

$$\vec{z} = f1(a, \vec{x}, \vec{y})$$

→

```
void f1(range1 i, double a, double* z,
            double* x, double* y)
{
            z[i] = a * x[i] + y[i];
}
```

Calls are generated as:

```
ParallelCall( f1, RangeOf(z), a, z, x, y);
```

FINAL CODE-GENERATION

- When all the conversions are ready the program tree is traversed and all the branch operators are converted to their textual equivalents in the selected languages.

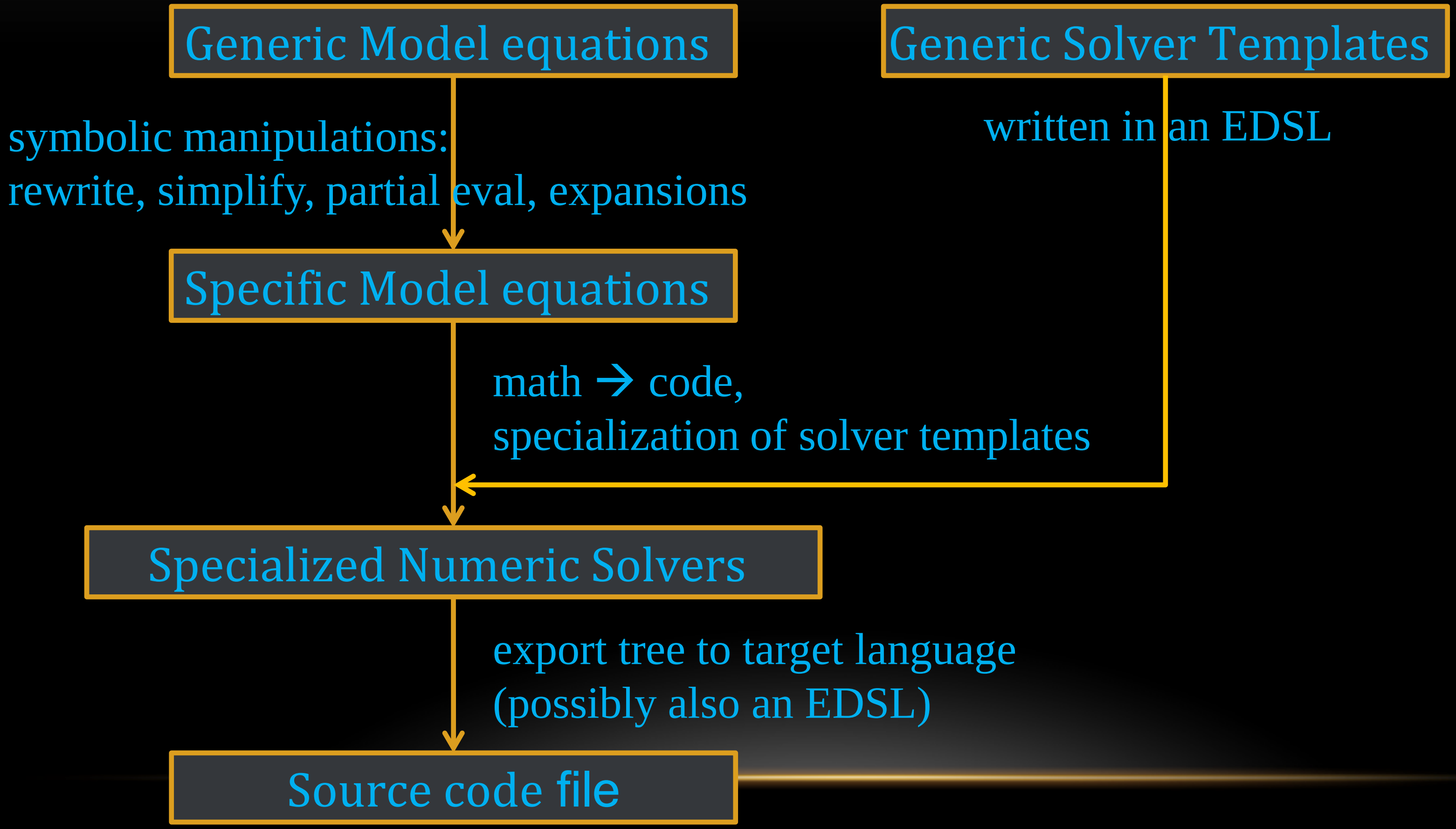
- Currently C++ / C / OpenCL export is considered.

  Why the C family?

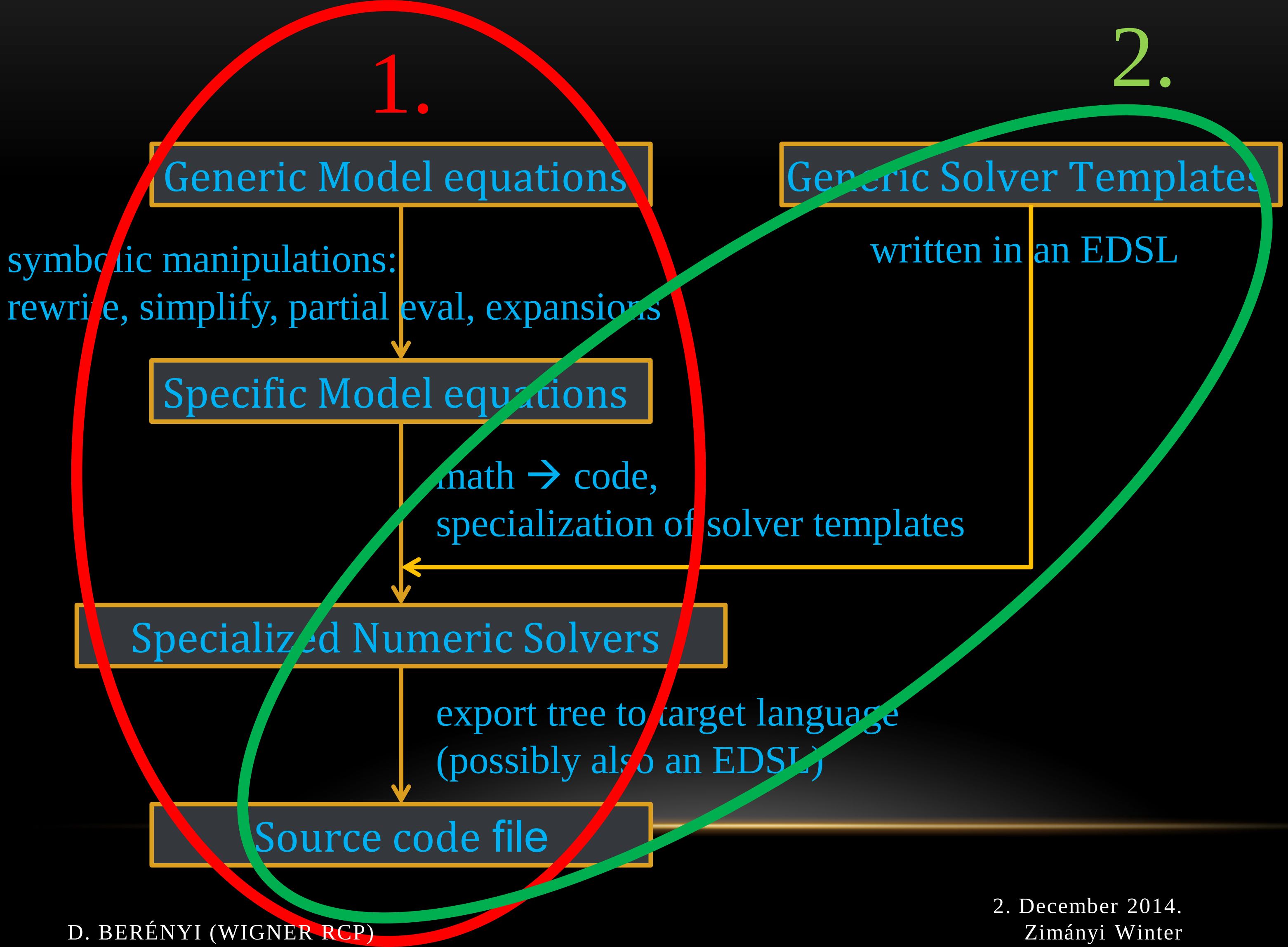
  Largest common set of features supported by the compute and rendering APIs:

  OpenCL kernel C, OpenGL GLSL, DirectCompute, DirectX HLSL

CODE-GENERATION FLOW



CODE-GENERATION FLOW



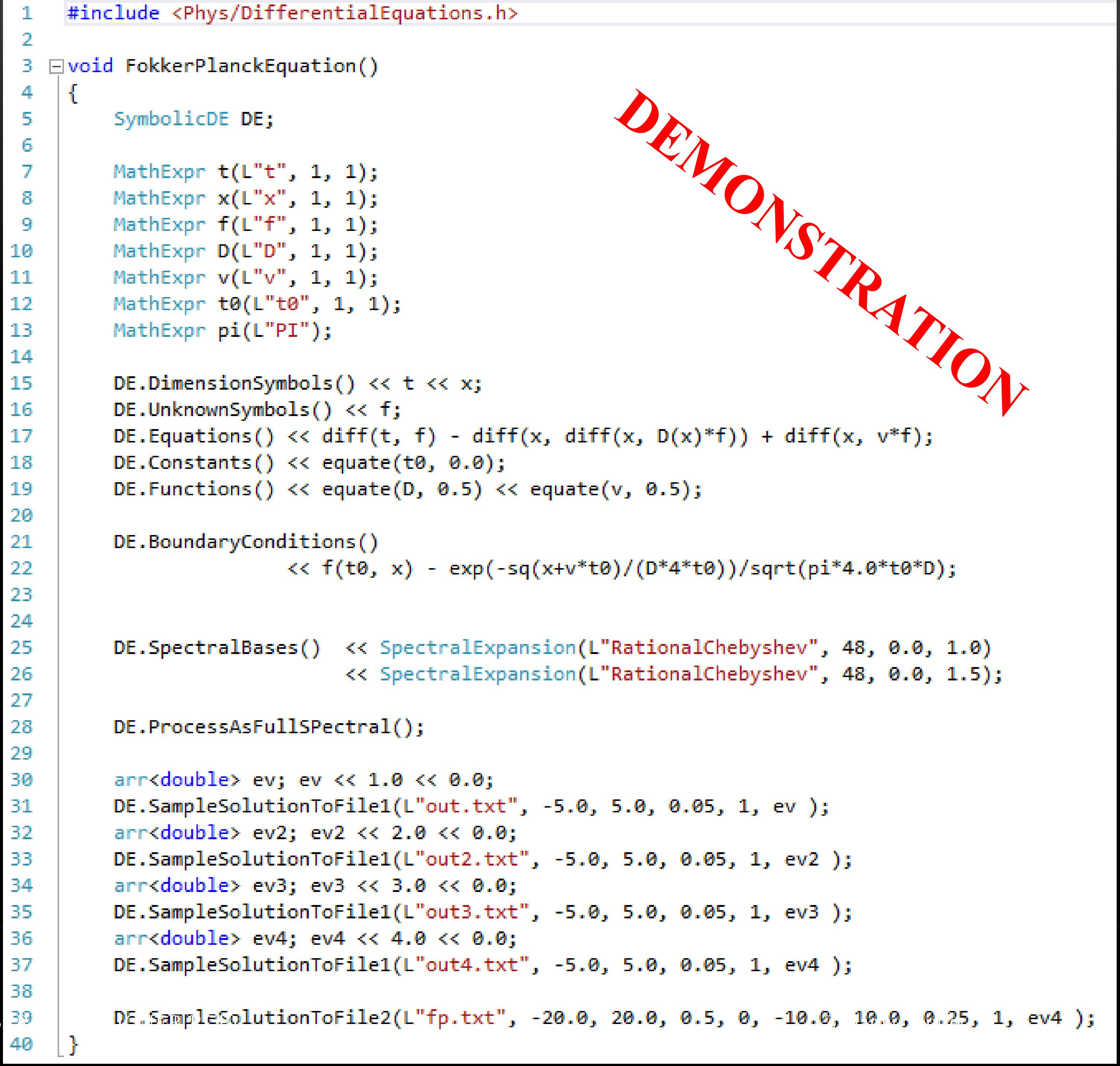
CURRENT IMPLEMENTATIONS

The above workflow has been splitted into two pilot projects:

1.: A full spectral solver for 1D / 2D DEs:

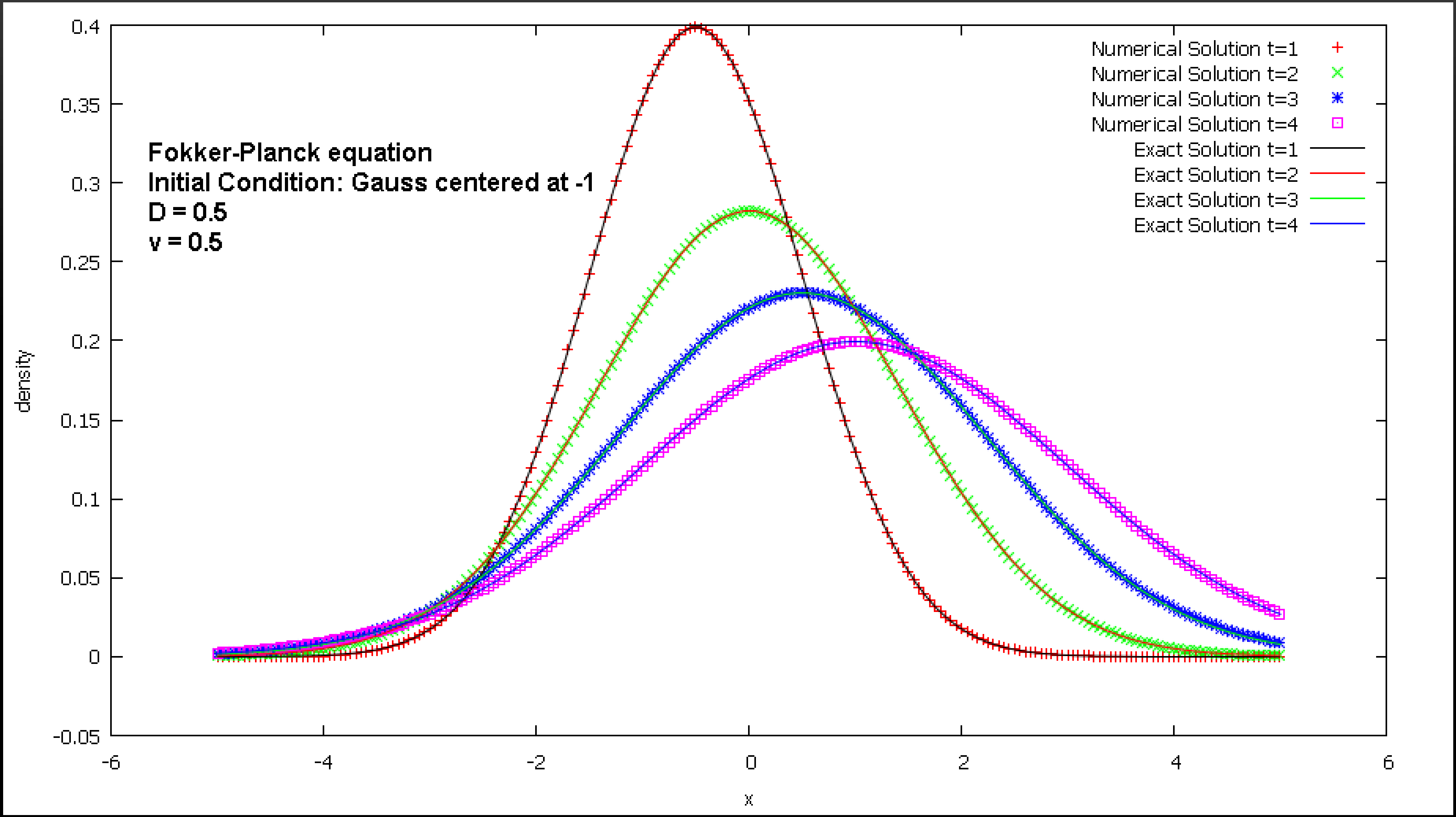
- Input of Equations, Variables and ranges in C++ code.
- Automatic symbolic simplification and spectral expansion
- Construction of the spectral coefficient matrix
- Inversion on the GPU (naïve non-generated LU decomposition)

Currently limited by the available memory on the GPU
(Further work: partition of the coefficient matrix)



```
#include <Phys/DifferentialEquations.h>

void FokkerPlanckEquation()
{
    SymbolicDE DE;

    MathExpr t(L"t", 1, 1);
    MathExpr x(L"x", 1, 1);
    MathExpr f(L"f", 1, 1);
    MathExpr D(L"D", 1, 1);
    MathExpr v(L"v", 1, 1);
    MathExpr t0(L"t0", 1, 1);
    MathExpr pi(L"PI");

    DE.DimensionSymbols() << t << x;
    DE.UnknownSymbols() << f;
    DE.Equations() << diff(t, f) - diff(x, diff(x, D(x)*f)) + diff(x, v*f);
    DE.Constants() << equate(t0, 0.0);
    DE.Functions() << equate(D, 0.5) << equate(v, 0.5);

    DE.BoundaryConditions()
               << f(t0, x) - exp(-sq(x+v*t0)/(D*4*t0))/sqrt(pi*4.0*t0*D);


    DE.SpectralBases()  << SpectralExpansion(L"RationalChebyshev", 48, 0.0, 1.0)
                        << SpectralExpansion(L"RationalChebyshev", 48, 0.0, 1.5);

    DE.ProcessAsFullSPectral();

    arr<double> ev; ev << 1.0 << 0.0;
    DE.SampleSolutionToFile1(L"out.txt", -5.0, 5.0, 0.05, 1, ev );
    arr<double> ev2; ev2 << 2.0 << 0.0;
    DE.SampleSolutionToFile1(L"out2.txt", -5.0, 5.0, 0.05, 1, ev2 );
    arr<double> ev3; ev3 << 3.0 << 0.0;
    DE.SampleSolutionToFile1(L"out3.txt", -5.0, 5.0, 0.05, 1, ev3 );
    arr<double> ev4; ev4 << 4.0 << 0.0;
    DE.SampleSolutionToFile1(L"out4.txt", -5.0, 5.0, 0.05, 1, ev4 );

    DE.SampleSolutionToFile2(L"fp.txt", -20.0, 20.0, 0.5, 0, -10.0, 10.0, 0.25, 1, ev4 );
}
```

DEMONSTRATION


Fokker-Planck equation
Initial Condition: Gauss centered at -1
D = 0.5
v = 0.5
Numerical Solution t=1
Numerical Solution t=2
Numerical Solution t=3
Numerical Solution t=4
Exact Solution t=1
Exact Solution t=2
Exact Solution t=3
Exact Solution t=4
density
x
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-6
-4
-2
0
2
4
6

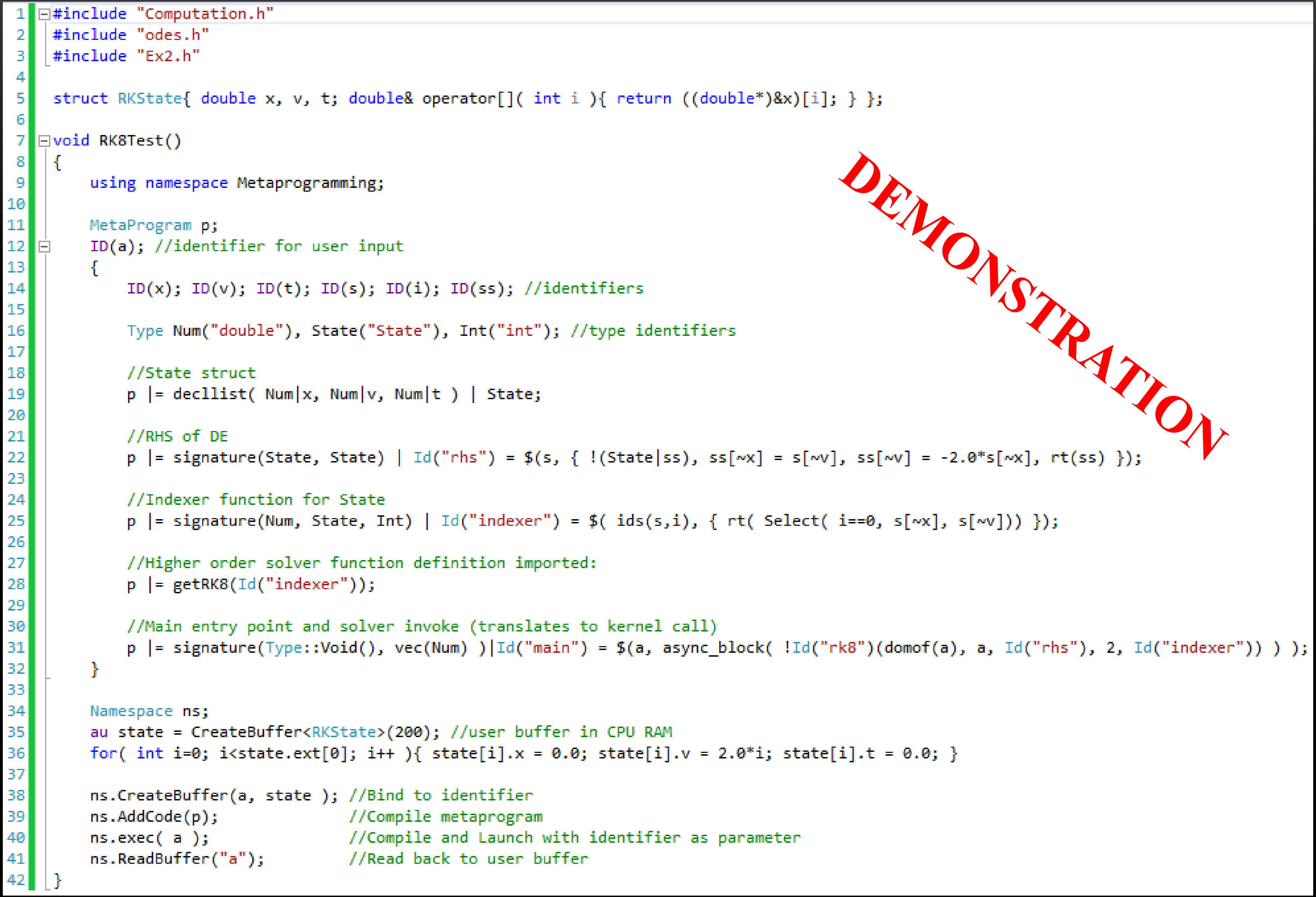
CURRENT IMPLEMENTATIONS

The above workflow has been splitted into two pilot projects:

2.: Host/Client OpenCL GPU code generator:

- A C like EDSL was created in C++ with wrapper classes
- An 8th order Runge-Kutta stepper was implemented in the EDSL
- The EDSL is manipulated:
  (defunctionalization, parallel call construction, host side C++ code and GPU side OpenCL Kernel generation)
- Then exported and compiled runtime into a DLL and loaded back to the program.
- A functor is supplied to the user to be called with data buffers and parameters.

  Successfully tested with simple ODEs.
  Asynchronous execution based on data dependency is currently being developed.



```cpp
#include "Computation.h"
#include "odes.h"
#include "Ex2.h"

struct RKState{ double x, v, t; double& operator[]( int i ){ return ((double*)&x)[i]; } };

void RK8Test()
{
    using namespace Metaprogramming;

    MetaProgram p;
    ID(a); //identifier for user input
    {
        ID(x); ID(v); ID(t); ID(s); ID(i); ID(ss); //identifiers

        Type Num("double"), State("State"), Int("int"); //type identifiers

        //State struct
        p |= decllist( Num|x, Num|v, Num|t ) | State;

        //RHS of DE
        p |= signature(State, State) | Id("rhs") = $(s, { !(State|ss), ss[~x] = s[~v], ss[~v] = -2.0*s[~x], rt(ss) });

        //Indexer function for State
        p |= signature(Num, State, Int) | Id("indexer") = $( ids(s,i), { rt( Select( i==0, s[~x], s[~v])) });

        //Higher order solver function definition imported:
        p |= getRK8(Id("indexer"));

        //Main entry point and solver invoke (translates to kernel call)
        p |= signature(Type::Void(), vec(Num) )|Id("main") = $(a, async_block( !Id("rk8")(domof(a), a, Id("rhs"), 2, Id("indexer")) ) );
    }

    Namespace ns;
    au state = CreateBuffer<RKState>(200); //user buffer in CPU RAM
    for( int i=0; i<state.ext[0]; i++ ){ state[i].x = 0.0; state[i].v = 2.0*i; state[i].t = 0.0; }

    ns.CreateBuffer(a, state ); //Bind to identifier
    ns.AddCode(p);              //Compile metaprogram
    ns.exec( a );               //Compile and Launch with identifier as parameter
    ns.ReadBuffer("a");         //Read back to user buffer
}
```

DEMONSTRATION

CURRENT STATUS

- In the case of a homogeneous electric field, the equation system is a 3 component ODE, it decouples in the momentum variable.
- In this case the 2. method was fully implemented (parallelized over the momentum variable).
- The resulting speed-up is around 30x
- The PDE solver is under development.