INTRODUCTION TO HIGH-LEVEL-SIMULATION LANGUAGE XMDS 2

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mpipks
Finite Systems

MAX-PLANCK-GESELLSCHAFT

HIGH-LEVEL APPROACH

```
    <![CDATA[
     double dens=phi.re*phi.re + phi.im*phi.im;

     dphi_dt =  L[phi] + x*Gy[phi] -y*Gx[phi]- i*(U*dens + trap )*phi;
  </operators>
</integrate>
```

- Human-readable equations
- No hassle with loops, array indices, libraries etc.

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="y" lattice="&Npts;"  domain="(-&L;, &L;)" />
  </transverse_dimensions>
</geometry>
```

- Easy addition of more PDE dimensions

```
<driver name="distributed-mpi" />
```

- Inbuilt parallel processing (MPI) support

```
<driver name="multi-path" paths="1000" />
```

- Inbuilt stochastic (P)DE solving and averaging

```
<noise_vector name="drivingNoise" kind="wiener" type="real" method="dsfmt">
  <components>dW</components>
</noise_vector>
```

COURSE OUTLINE

1) XMDS basics (simple example, XML script, main tags)

2) Exercise one (xmds basics, 1D Gross-Pitaevskii equation)

3) XMDS advanced (advanced examples, parallel code, stochastic DEs, ...)

4) Exercise two (stochastic sims, kink-bearing phi^4 theory)

5) Hacking XMDS

LUNCH

6) Exercise three (Code your own problem)

DISCLAIMER

Course targets:

- Enable you to straightaway start working with XMDS
- Enable you to assess whether XMDS suits your problem
- Provide you with some small bits-and-pieces of: XML, C, numerical algorithms, cold-atomic-physics, PDEs to illustrate things.

Not course targets:

- Enable you to use XML or C or C++ beyond what is needed for XMDS.
- Teach you the numerical propagation algorithms employed by XMDS in any detail.
- Teach the physics of all the numerical examples

XMDS BASICS

simple example (exercise zero)

file derived from: examples/sech_soliton.xmds

- Nonlinear Schrödinger equation (NLSE)

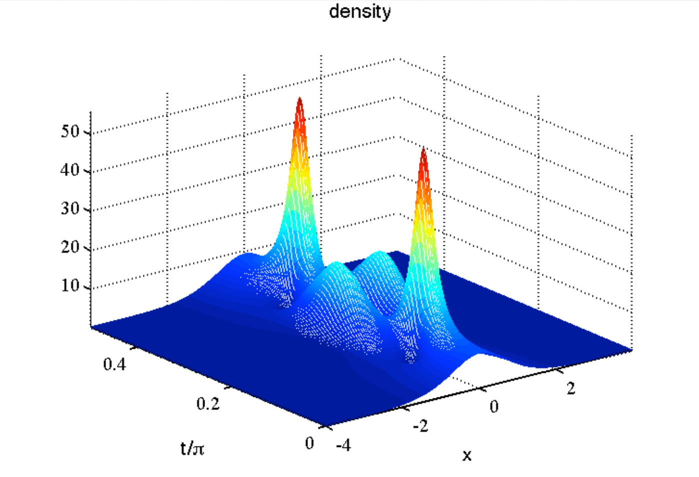
$$i\frac{d\psi}{dt} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi - |\psi|^2\psi$$

- Solution

$$\psi(x,t)$$

- Breathing soliton reforms precisely after period pi/2 (for N>1, N=1 stationary)

$$\psi(x,t=0) = \frac{N}{\cosh x}$$



HEADER

```
<simulation xmds-version="2">
  <name>sech_soliton</name>

  <author>Sebastian Wuester / Graham Dennis</author>
  <description>
    Nonlinear Schrodinger equation with attractive interactions.
    This equation has an analytic solution of the form of a breathing soliton.
  </description>

  <geometry>
    <propagation_dimension> t </propagation_dimension>
    <transverse_dimensions>
      <dimension name="x" lattice="4096"  domain="(-4.0, 4.0)" />
    </transverse_dimensions>
  </geometry>

  <features>
    <auto_vectorise />
    <fftw />
    <globals>
      <![CDATA[
      const double N = 3.0;
      ]]>
    </globals>
  </features>

              ●●●●●

</simulation>
```

- Edit existing XML script
- Header of script:
  Name
  Geometry (PDE or ODE ?)
- Steering (features, parameters)

HEADER

```
<simulation xmds-version="2">
  <name>sech_soliton</name>

  <author>Sebastian Wuester / Graham Dennis</author>
  <description>
    Nonlinear Schrodinger equation with attractive interactions.
    This equation has an analytic solution of the form of a breathing soliton.
  </description>

  <geometry>
    <propagation_dimension> t </propagation_dimension>
    <transverse_dimensions>
      <dimension name="x" lattice="4096"  domain="(-4.0, 4.0)" />
    </transverse_dimensions>
  </geometry>

  <features>
    <auto_vectorise />
    <fftw />
    <globals>
      <![CDATA[
      const double N = 3.0;
      ]]>
    </globals>
  </features>
```

●●●●●

$$\psi(x, t=0) = \frac{N}{\cosh x}$$

```
</simulation>
```

- Edit existing XML script
- Header of script:
  Name
  Geometry (PDE or ODE ?)
- Steering (features, parameters)

INITIALISATION

```
        •••••
</features>

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
      psi = N/cosh(x);
    ]]>
  </initialisation>
</vector>
```

$$\psi(x, t = 0) = \frac{N}{\cosh x}$$

- <vector> tag, defines:
- solution function
- multi-component solution vectors
- parameter type functions appearing in PDE (e.g. potential)

INITIALISATION

```
        •••••
</features>

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
      psi = N/cosh(x);
    ]]>
  </initialisation>
</vector>
```

$$\psi(x, t = 0) = \frac{N}{\cosh x}$$

- <vector> tag, defines:
- solution function
- multi-component solution vectors
- parameter type functions appearing in PDE (e.g. potential)

SOLVER

```
   ●●●●●
</vector>

<sequence>
  <integrate algorithm="ARK45" interval="1.570796327" tolerance="1e-6">
    <samples>200</samples>
    <operators>
      <operator kind="ip">
        <operator_names>L</operator_names>
        <![CDATA[
          L = -0.5*i*kx*kx;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <![CDATA[
        dpsi_dt = L[psi] + i*mod2(psi)*psi;
      ]]>
    </operators>
  </integrate>
</sequence>
```

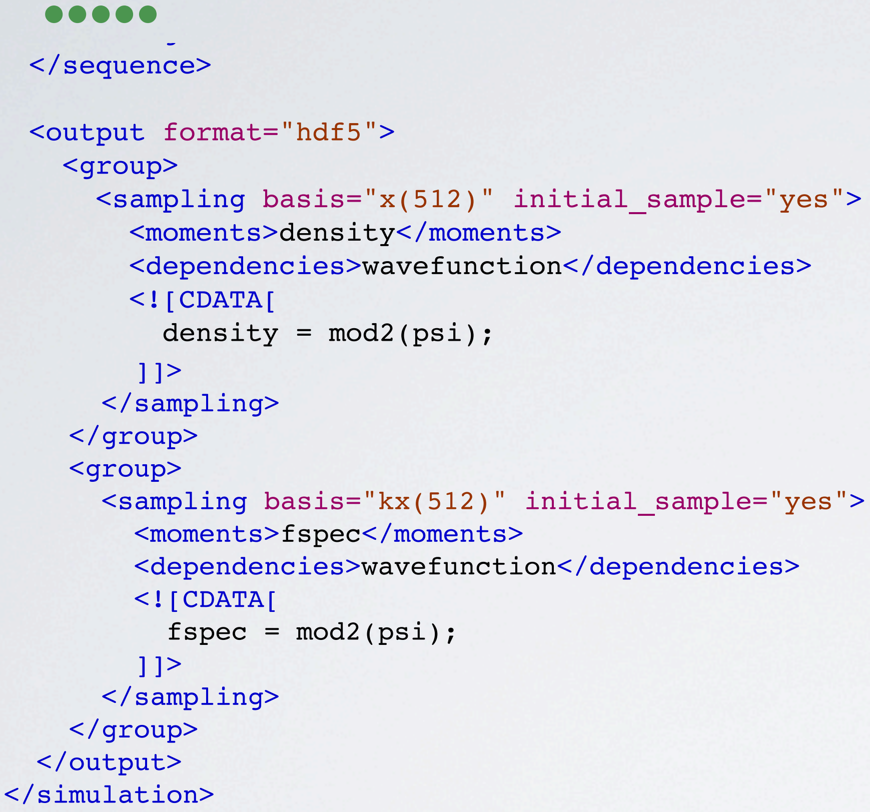
- All calculations contained in top-level <sequence>

- <integrate> is main calculation/DE solver block

- <sequence> can contain sub-sequences, these are then loops.

- Top-level sequence can contain also, e.g. <filter>

OUTPUT



```
  </sequence>

  <output format="hdf5">
    <group>
      <sampling basis="x(512)" initial_sample="yes">
        <moments>density</moments>
        <dependencies>wavefunction</dependencies>
        <![CDATA[
          density = mod2(psi);
        ]]>
      </sampling>
    </group>
    <group>
      <sampling basis="kx(512)" initial_sample="yes">
        <moments>fspec</moments>
        <dependencies>wavefunction</dependencies>
        <![CDATA[
          fspec = mod2(psi);
        ]]>
      </sampling>
    </group>
  </output>
</simulation>
```

- write binary, ascii or hdf5
- export that data to matlab
- sample all or some (for large simulations) of accumulated data
- do some processing on output already at code level (e.g. sample Fourier spectrum)
- takes *real part* only

RUNNING

- invoke code generator:

  ```
  xmds2 sech_soliton.xmds
  ```

- writes and compiles c-code,
  filenames taken from <name>

  ```
  → sech_soliton.cc
  → sech_soliton
  ```

- run or submit code as usual

  ```
  ./sech_soliton
  ```

READING OUTPUT

- After execution we have files:

```
-rw-r--r-- 1 sew654 mks    1895 2011-12-27 22:44 sech_soliton_course.xmds
-rw-r--r-- 1 sew654 mks   66301 2011-12-27 22:44 sech_soliton.cc
-rwxr-xr-x 1 sew654 mks   81886 2011-12-27 22:44 sech_soliton
-rw-r--r-- 1 sew654 mks 1673792 2011-12-27 22:44 sech_soliton.h5
-rw-r--r-- 1 sew654 mks    2853 2011-12-27 22:44 sech_soliton.xsil
```

- h5 contains data. xsil contains metadata AND also includes the XMDS script for reference

```
xsil2graphics2  sech_soliton.xsil
  ⟶ sech_soliton.m
```

```
-rw-r--r-- 1 sew654 mks     384 2011-12-27 22:44 sech_soliton.m
```

- generate matlab import script for output

```
matlab -nodesktop
sech_soliton
```

- import data into e.g. matlab

MORE ON GEOMETRY

```
<geometry>
    <propagation_dimension> t </propagation_dimension>
    <transverse_dimensions>
        <dimension name="z" lattice="1024"  domain="(-100,100)" />
        <dimension name="y" lattice="256"  domain="(-10,10)" />
        <dimension name="x" lattice="256"  domain="(-10,10)" />
        <dimension name="j" type="integer" lattice="8" domain="(0,7)" aliases="k"/>
    </transverse_dimensions>
 </geometry>
```

- Multi-dimensional simulations => more transverse dimensions
- Dimension with most grid-points first, case we ever need MPI
- Can also have discrete dimensions (e.g. internal states of atom)
- Example above: $i\dfrac{d\psi_j(x,y,z)}{dt} = F[\psi_k(x,y,z)]$
- *(More about integer dimensions in advanced part)*

MORE ON VECTORS

```
</features>

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
      psi = N/cosh(x);
    ]]>
  </initialisation>
</vector>
```

define initial-state in Fourier-space

```
  <vector name="wavefunction" initial_space="kx" type="complex">
  <components>phi psi</components>
  <initialisation>
    <![CDATA[
       const double delkx = kx - kx0;
       phi = norm*exp(-0.5*delkx*delkx/sigmak/sigmak);

       psi = 0.0;
    ]]>
  </initialisation>
</vector>
```

vector with two different components

```
<vector name="potentials" dimensions="x" type="real">
  <components> barrier </components>
  <evaluation>
    <![CDATA[
      barrier = 0.0;
      if( (x>0)&&(x<1) )
         barrier = V0;
    ]]>
  </evaluation>
</vector>
```

save memory and computation time if data is real

like, this, compute only once at beginning

```
<sequence>
<integrate algorithm="rk4" interval="300" steps="10000">

  <integration_vectors> wavefunction </integration_vectors>
  <dependencies> potentials </dependencies>
```

MORE ON VECTORS II

```
</features>

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
      psi = N/cosh(x);
    ]]>
  </initialisation>
</vector>
```

```
<computed_vector name="moments" dimensions="" type="real">
  <components> norm meanx </components>
  <evaluation>
    <dependencies  basis="x"> wavefunction </dependencies>
    <![CDATA[
       norm =  mod2(phi);
       meanx = x*mod2(phi);
    ]]>
  </evaluation>
</computed_vector>
```

Computed vector:
- NOT stored,
- only calculated when needed

If #dim dependencies> #dim vector
surplus dimensions are integrated out

MORE ON INTEGRATE

```
</vector>

<sequence>
  <integrate algorithm="ARK45" interval="1.570796327" tolerance="1e-6">
    <samples>200</samples>
    <operators>
      <operator kind="ip">
        <operator_names>L</operator_names>
        <![CDATA[
          L = -0.5*i*kx*kx;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <![CDATA[
        dpsi_dt = L[psi] + i*mod2(psi)*psi;
      ]]>
    </operators>
  </integrate>
</sequence>
```

fixed step algorithm

```
<integrate algorithm="rk4" interval="300" steps="10000">
  <samples>200 200 200 200 200</samples>
  <operators>
    <operator kind="ex">
      <operator_names>L Gy Gx</operator_names>
      <![CDATA[
       L = rcomplex(0,-kx*kx/2.0 -ky*ky/2.0);
       Gy =rcomplex(0,Omega*ky);
       Gx =rcomplex(0,Omega*kx);
      ]]>
    </operator>
    <integration_vectors>wavefunction</integration_vectors>
    <dependencies>potentials</dependencies>
    <![CDATA[
     double dens=phi.re*phi.re + phi.im*phi.im;

     dphi_dt =  L[phi] + x*Gy[phi] -y*Gx[phi]- i*(U*dens + barrier )*phi - i*kappa*psi;
     dpsi_dt =  L[psi] + x*Gy[psi] -y*Gx[psi]- i*(U*dens)*psi - i*kappa*phi;
     ]]>
  </operators>
</integrate>
```

samples for *each* output group

use constant vector

explicit derivatives, MUST use for products of co-ordinates and derivatives

MORE ON ALGORITHMS

- available time-stepping algorithms:
  "ark89" adaptive stepsize, 8th/ 9th order Runge-Kutta,
  "ark45" adaptive stepsize, 4th/ 5th order Runge-Kutta,
  "rk4" fixed stepsize, 4th order Runge-Kutta,
  "si" semi-implicit algorithm for stochastic problems

- For PDEs, all these come in

  the "ip" (interaction picture)
  (split-step, for Runge-Kutta)

  or "ex" (explicit) version

$$\frac{\partial}{\partial x} f \to \mathcal{F}^{-1}[ik\mathcal{F}[f]]$$

$$i\frac{d\psi}{dt} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi + V(x) + U|\psi|^2\psi$$

(split-step, for Euler scheme)

$$\psi(x,t+\Delta t) \overset{\mathcal{F}^{-1}}{\longleftarrow} e^{[-\frac{k^2\Delta t}{4}]}\psi(k,t)$$

$$\overset{\mathcal{F}}{\longleftarrow}$$

$$[\psi(x,t) + (V(x) + U|\psi(x,t)|^2\psi(x,t))\Delta t]$$

$$\overset{\mathcal{F}^{-1}}{\longleftarrow}$$

$$e^{[-\frac{k^2\Delta t}{4}]}\psi(k,t) \overset{\mathcal{F}}{\longleftarrow} \psi(x,t)$$

ERROR CHECKING

- Numerical solution, always have to check for convergence

```
<features>
  <error_check />
</features>
```

```
.......
Generating output for GPE_1D_course
Maximum step error in moment group 1 was 8.905735e-04
Maximum step error in moment group 2 was 4.287776e-15
Maximum step error in moment group 3 was 3.622347e-11
Time elapsed for simulation is: 0.28 seconds
```

- Simulation will run once with stepsize dt = Tmax/Nsteps and once with dt'=dt/2. (or for adaptive step-size once with tolerance tol, and once with tolerance tol/16 (for fourth order method).

```
density_1
fspec_2
atomnumber_3

error_density_1
error_fspec_2
error_atomnumber_3
```

- Little aside: this is an XML comment:

```
<!-- this line is a comment -->
```

EXERCISE ONE

- 1D Gross-Pitaevskii equation (BEC in harmonic trap)

$$i\hbar\frac{d\psi}{dt} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 + U_{1D}|\psi|^2\right]\psi$$

- Parameters

$$\hbar = 1.05457266 \times 10^{-34}$$
$$m = 1.4432 \times 10^{-25}$$
$$a_s = 5.5\,\text{e-9}$$
$$\omega = 10 \times (2\pi)$$

$$U = \frac{4\pi\hbar^2 a_s}{m}$$
$$U_{1D} = U/(2\pi\sigma_\perp^2)$$
$$\omega_\perp = 200 \times (2\pi)$$

- Initial state

$$\mathcal{N}\exp\left[-(x-x_0)^2/2/\sigma^2\right]$$
$$\mathcal{N} = \sqrt{N}/(\pi\sigma^2)^{1/4}$$

$$\sigma = \sqrt{\frac{\hbar}{m\omega}}$$
$$N = 100$$

- Simulated domain and time

$$X_{max} = 30\mu m$$
$$T_{max} = 0.4s$$

EXERCISE ONE

List of tasks

- Edit simulation: add harmonic trap, use SI units
- Run XMDS, run code, import data into matlab
- Plot some output
- Verify normalisation by sampling $N = \int dx |\psi|^2$
- Determine breathing frequency by sampling

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\int dx\; x^2 |\Psi|^2 / N - \left(\int dx\; x |\Psi|^2 / N \right)^2}$$

XMDS ADVANCED

- XML-shortcuts, MPI-parallelisation, filter, breakpoints, load from file
- Random noise, multi-paths, averaged output, mpi-multi-paths, SDEs
- Command line parameters, discrete dimensions, basis change, convolution
- Exercise II: Kink-bearing phi^4 field theory, stochastic simulation

XML SHORTCUTS

from solution to exercise one: GPE_1D_course.xmds

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE simulation [
<!ENTITY Npts      "64">
<!ENTITY Nsamples    "64">
<!ENTITY L  "3e-5">
]>
<simulation xmds-version="2">
  <name>GPE_1D_course</name>
```

define XML "variables"

●●●●●

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
  </transverse_dimensions>
</geometry>
```

ensure symmetric grid

●●●●●

```
  <group>
    <sampling basis="x(&Nsamples;)" initial_sample="yes">
      <moments>density phire phiim trappotential interaction_term</moments>
      <dependencies>wavefunction potentials</dependencies>
      <![CDATA[
        density = mod2(phi);
        phire = phi.Re();
        phiim = phi.Im();
        trappotential = trap;
        interaction_term = U1d*mod2(phi);
      ]]>
    </sampling>
  </group>
  <group>
    <sampling basis="kx(&Npts;)" initial_sample="yes">
      <moments>fspec</moments>
      <dependencies>wavefunction</dependencies>
      <![CDATA[
        fspec = mod2(phi);
      ]]>
```

●●●●●

this example makes sure we always sample full Fourier space

PARALLELISATION

```
<geometry>
    <propagation_dimension> t </propagation_dimension>
    <transverse_dimensions>
        <dimension name="z" lattice="1024"  domain="(-100,100)" />
        <dimension name="y" lattice="256"  domain="(-10,10)" />
        <dimension name="x" lattice="256"  domain="(-10,10)" />
        <dimension name="j" type="integer" lattice="8" domain="(0,7)" aliases="k"/>
    </transverse_dimensions>
 </geometry>
```

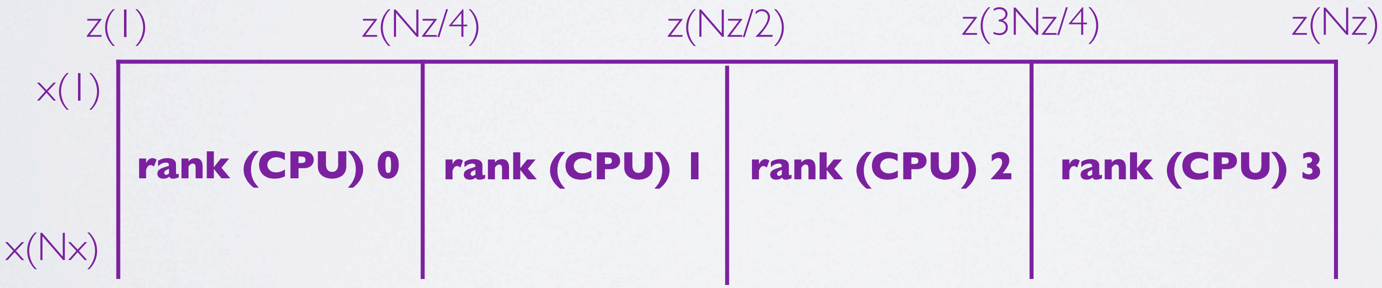
- 2D/3D-multicomponent simulations can benefit from parallelisation
- XMDS parallelises with one line:

```
<driver name="distributed-mpi" />
```

or

```
<features>
  <openmp />
  <globals>
    <![CDATA[
```

- MPI: Slab decomposition along first dimension (that should be the largest)



z(1) z(Nz/4) z(Nz/2) z(3Nz/4) z(Nz)

x(1)

x(Nx)

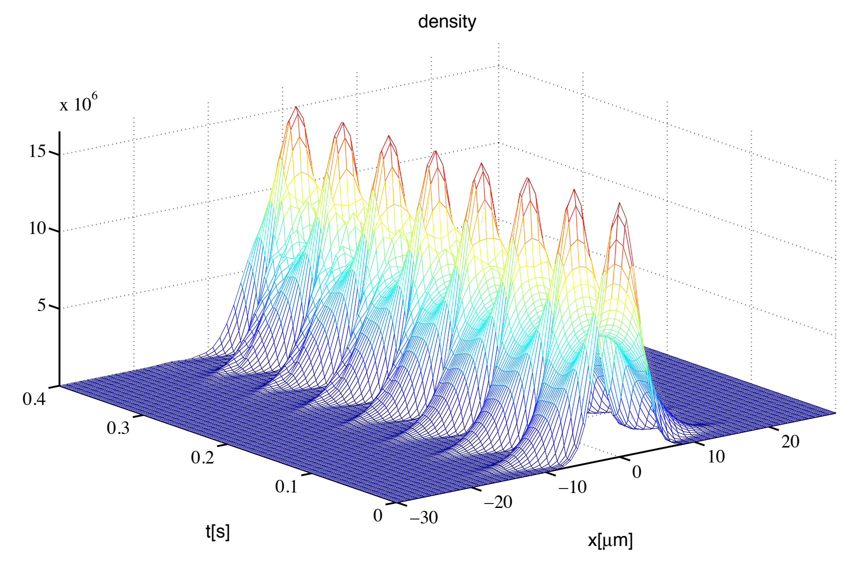
rank (CPU) 0 **rank (CPU) 1** **rank (CPU) 2** **rank (CPU) 3**

- Will then need mpi jobscripts (see example)

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#wignerarguments

FILTERS

- Seen breathing oscillations in first example:



- Find Groundstate of: 1D Gross-Pitaevskii equation using **imaginary time evolution**

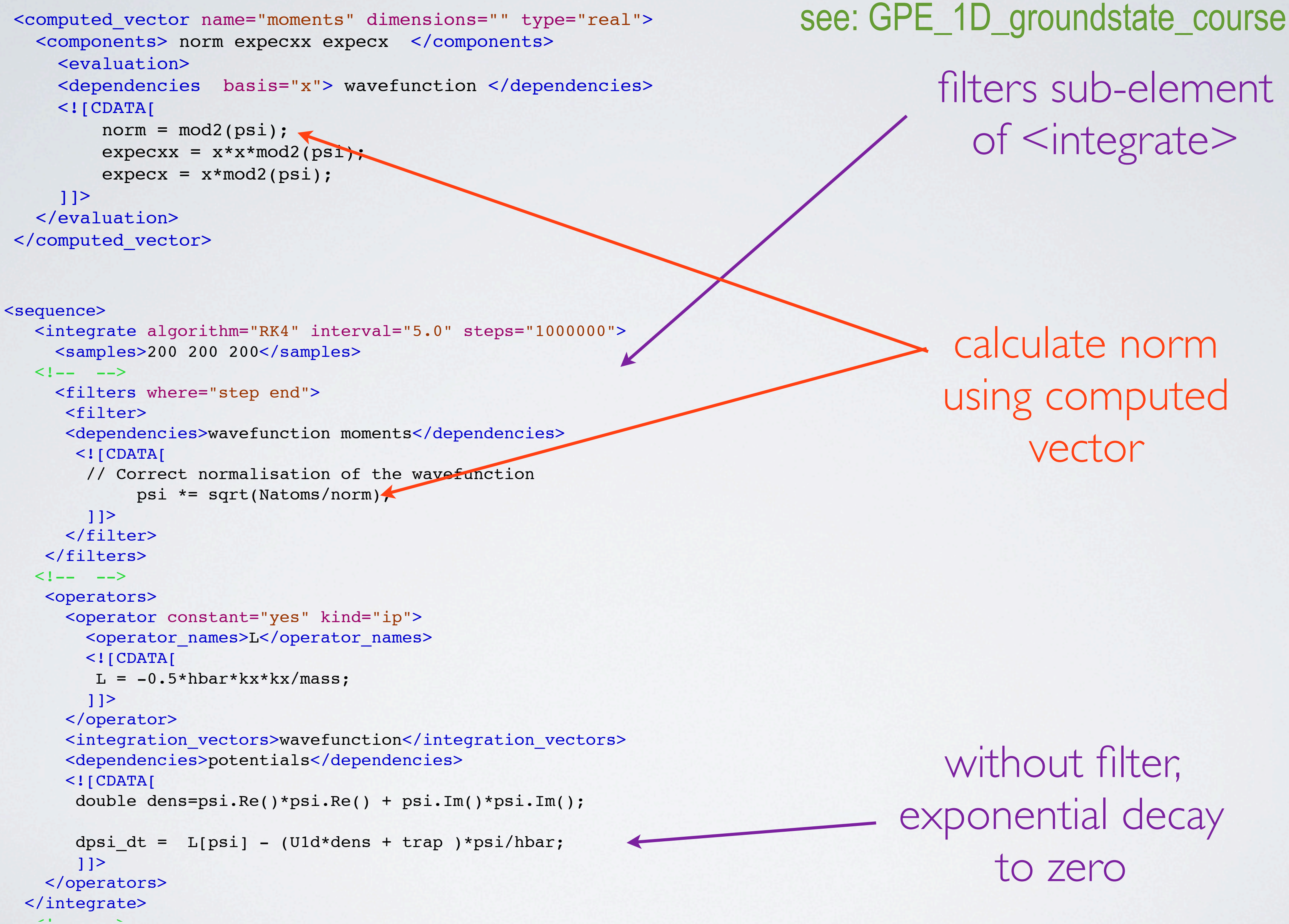
$$\hbar\frac{d\psi}{d\tau} = -\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 + U|\psi|^2\right]\psi$$

- Need to fix norm of wave function

$$\int dx|\psi|^2 = N$$

FILTERS

see: GPE_1D_groundstate_course.xmds



```
<computed_vector name="moments" dimensions="" type="real">
  <components> norm expecxx expecx  </components>
    <evaluation>
    <dependencies  basis="x"> wavefunction </dependencies>
    <![CDATA[
        norm = mod2(psi);
        expecxx = x*x*mod2(psi);
        expecx = x*mod2(psi);
    ]]>
  </evaluation>
</computed_vector>


<sequence>
   <integrate algorithm="RK4" interval="5.0" steps="1000000">
     <samples>200 200 200</samples>
   <!--  -->
     <filters where="step end">
      <filter>
      <dependencies>wavefunction moments</dependencies>
       <![CDATA[
        // Correct normalisation of the wavefunction
             psi *= sqrt(Natoms/norm);
        ]]>
      </filter>
    </filters>
   <!--  -->
    <operators>
      <operator constant="yes" kind="ip">
        <operator_names>L</operator_names>
        <![CDATA[
         L = -0.5*hbar*kx*kx/mass;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <dependencies>potentials</dependencies>
      <![CDATA[
       double dens=psi.Re()*psi.Re() + psi.Im()*psi.Im();

       dpsi_dt =  L[psi] - (U1d*dens + trap )*psi/hbar;
       ]]>
    </operators>
  </integrate>
```

●●●●●

filters sub-element
of <integrate>

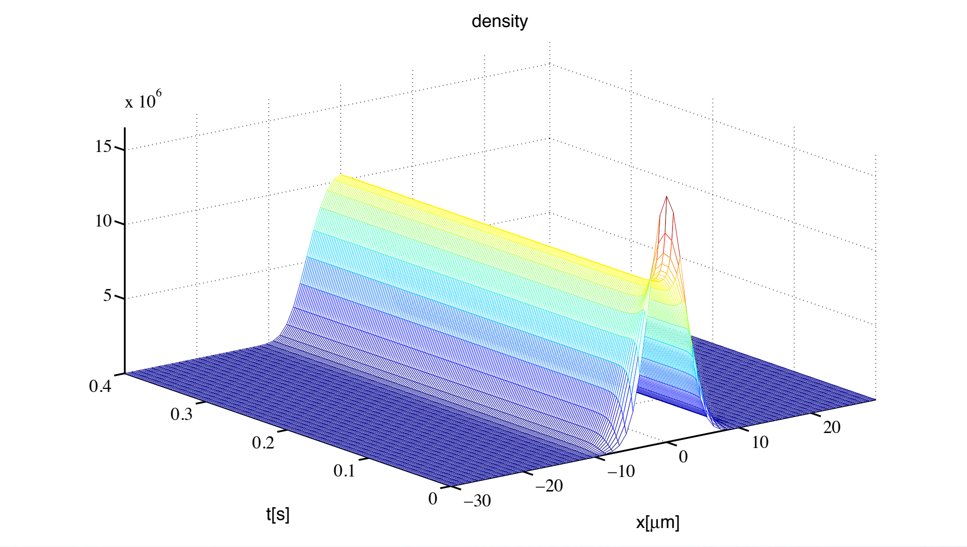
calculate norm
using computed
vector

without filter,
exponential decay
to zero

see also http://xmds2.readthedocs.org/en/latest/
worked_examples.html#groundstatebec

BREAKPOINTS

```
●●●●●
<sequence>
   <integrate algorithm="RK4" interval="5.0" steps="1000000">
     <samples>200 200 200</samples>
   <!--  -->
     <filters where="step end">
      <filter>
      <dependencies>wavefunction moments</dependencies>
       <![CDATA[
        // Correct normalisation of the wavefunction
             psi *= sqrt(Natoms/norm);
        ]]>
      </filter>
    </filters>
   <!--  -->
    <operators>
      <operator constant="yes" kind="ip">
        <operator_names>L</operator_names>
        <![CDATA[
         L = -0.5*hbar*kx*kx/mass;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <dependencies>potentials</dependencies>
      <![CDATA[
       double dens=psi.Re()*psi.Re() + psi.Im()*psi.Im();

       dpsi_dt =  L[psi] - (U1d*dens + trap )*psi/hbar;
       ]]>
    </operators>
  </integrate>
   <!--  -->
   <breakpoint filename="groundstate_break" format="hdf5">
    <dependencies basis="x"> wavefunction </dependencies>
  </breakpoint>
    <!--  -->
</sequence>
```



Write chosen vector to file, for continuation of simulation

Writes file: groundstate_break.h5

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#groundstatebec

LOAD FROM FILE

see: GPE_1D_stationary_course.xmds

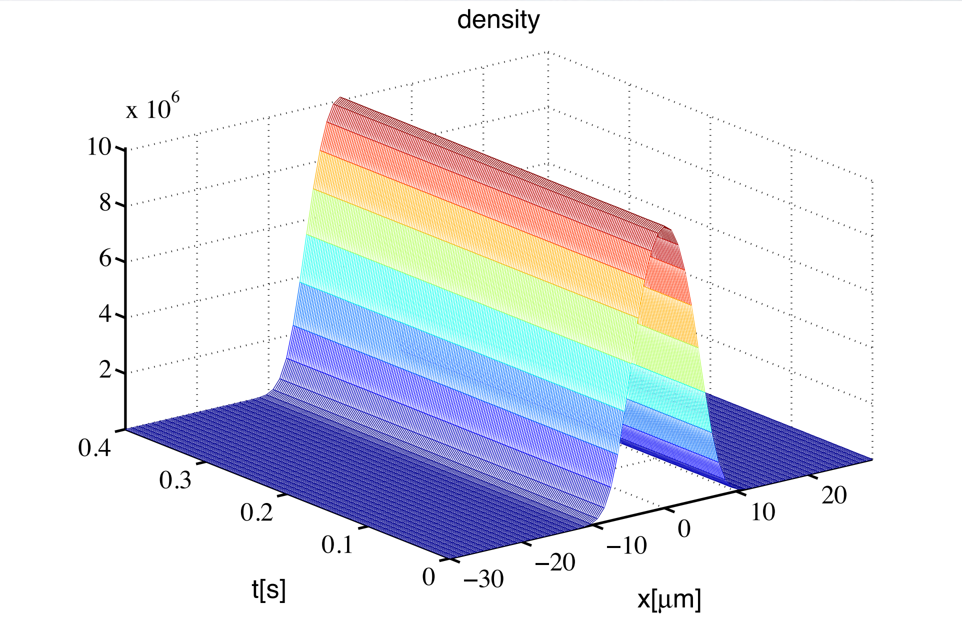
see: GPE_1D_allinone_course.xmds

- Load into dynamical (real time) simulation
- Confirm stationarity
- Can also load data generated in other ways (matlab, mathematica, text editor)
- Formats: ascii, hdf5, xsil

●●●●●

```
<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
<initialisation kind="hdf5">
  <filename> groundstate_break.h5</filename>
</initialisation>
</vector>
```

●●●●●



RANDOM NOISE

see: GPE_1D_noisy_course.xmds

```
<noise_vector name="thermalNoise" dimensions="x" kind="Gaussian"
              type="complex" method="dsfmt" seed="314 159 276">
  <components>Eta</components>
</noise_vector>
```

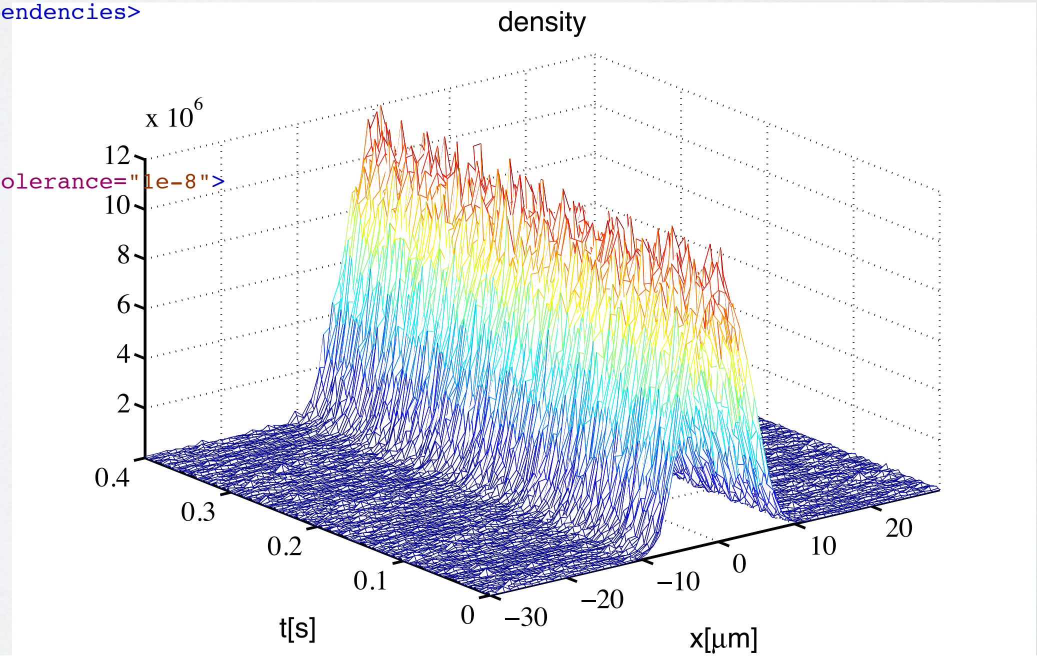
Dynamic: Wiener, Jump
Static: Uniform, Gaussian, Poissonian

noise generation
algorithm: mkl, dsfmt,
posix(default), solirte

seed: Reproducible
stochastic simulations,
leave empty to have
seed scrambled at
compile time

```
<sequence>
  <!--  -->
  <filter>
   <dependencies>wavefunction thermalNoise</dependencies>
   <![CDATA[
         psi += noiseamp*Eta;
     ]]>
  </filter>
  <!--  -->
  <integrate algorithm="ARK89" interval="0.4" tolerance="1e-8">
    <samples>200 200 200</samples>
    <operators>
```

filter can also be
sub-element of
<sequence>
(only done once)



MULTI-PATH/ AVERAGING

●●●●●

see: GPE_1D_noisy_course_MT.xmds

```
    ]]>
  </globals>
</features>

<driver name="multi-path" paths="100" />

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
<initialisation kind="hdf5">
```

Run simulation 100 times, automatically calculate averages and stderr

●●●●●

```
<noise_vector name="thermalNoise" dimensions="x" kind="Gaussian"
               type="complex" method="dsfmt" seed="314 159 276">
  <components>Eta</components>
</noise_vector>
```

Seed now valid only initially for all 100 runs

●●●●●

```
        -
</sequence>

<output format="hdf5">
  <group>
    <sampling basis="x(512)" initial_sample="yes">
      <moments>density</moments>
      <dependencies>wavefunction</dependencies>
      <![CDATA[
        density = mod2(psi);
```

variable A

Output variables: density_1 ==>mean_density_1,
stderr_density_1

definition: <A>

$$\sqrt{\frac{\langle AA\rangle - \langle A\rangle\langle A\rangle^2}{N_{trajs}}}$$

MULTI-PATH/ AVERAGING

●●●●●

```
    ]]>
  </globals>
</features>

<driver name="multi-path" paths="100" />

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
<initialisation kind="hdf5">
```

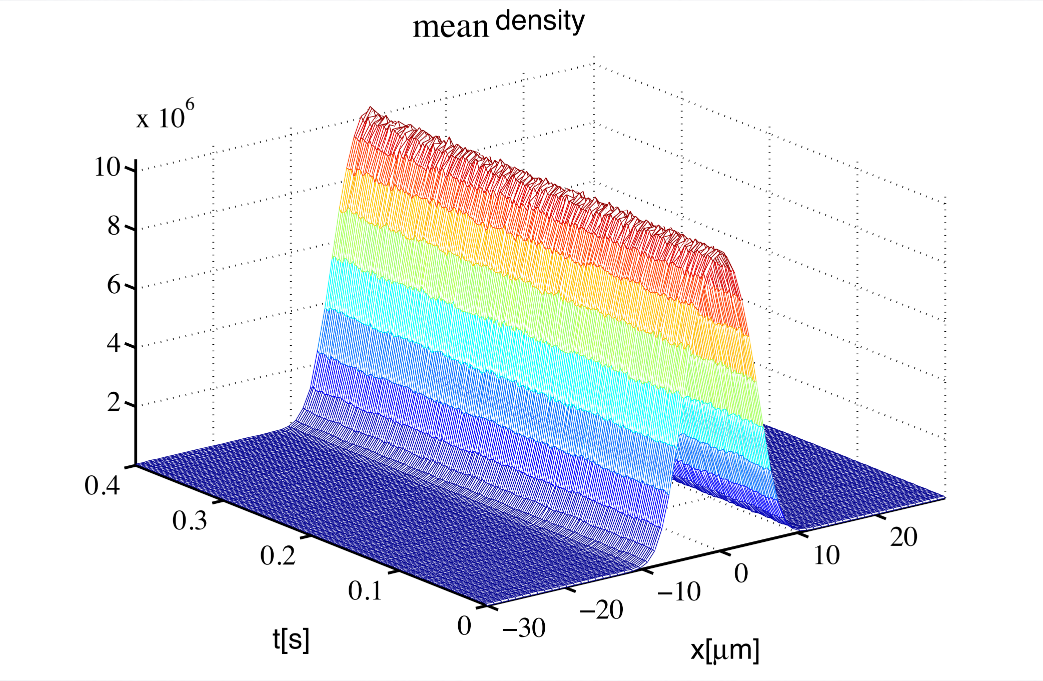
●●●●●

Run simulation 100 times, automatically calculate averages and stderr

Output variables: **A** density_1 ==>mean_density_1, stderr_density_1

<A>

Sqrt[(<AA>-<A><A>)/Npaths]



PARALLEL MULTI-PATH

```
<driver name="multi-path" paths="1000" />
```

Only small addition: Go from small sample to large sample, parallel processed

```
<driver name="mpi-multi-path" paths="640" />
```

Npaths, should be multiple of Ncpus

```
•••••
Rank[44]: Starting path 109
Rank[46]: Starting path 111
Rank[35]: Starting path 100
Rank[59]: Starting path 124
Rank[36]: Starting path 101
Rank[1]: Starting path 66
Rank[30]: Starting path 95
Rank[50]: Starting path 115
Rank[15]: Starting path 80
Rank[57]: Starting path 122
Rank[45]: Starting path 110
Rank[51]: Starting path 116
Rank[40]: Starting path 105
Rank[23]: Starting path 88
•••••
```

STOCHASTIC DE

- Langevin equation for brownian motion:

see: brownian_motion_course.xmds

$$m\frac{\partial^2 x}{\partial t^2} = -\lambda\frac{\partial x}{\partial t} + \eta(t)$$

$$\langle\eta(t)\eta(t')\rangle = 2\lambda T\delta(t-t')$$

```
const double noiseamp = sqrt(2.0*damping*Temperature);
```

●●●●●

```
<driver name="multi-path" paths="10000" />
```

●●●●●

```
<noise_vector name="drivingNoise" kind="Wiener" type="real" method="dsfmt" seed="23 42 1"
  <components>dW</components>
</noise_vector>
```

●●●●●

```
<sequence>
  <integrate algorithm="SI" interval="3" steps="10000">
    <samples>200 200 200</samples>
    <operators>
      <integration_vectors>variables </integration_vectors>
      <dependencies>drivingNoise</dependencies>
        <![CDATA[

          dpos_dt = vel;
          dvel_dt = -damping/mass*vel + noiseamp/mass*dW;
        ]]>
    </operators>
  </integrate>
</sequence>
```

Dynamical noise on each timestep

Algorithms converge against Stratonovich integral, for solving Ito SDE have to convert!!!

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#kubo

DISTRIBUTION SAMPLING

see: brownian_motion_course_MT.xmds

- Suppose we want to sample the position and velocity distribution functions p(x), p(v) [1D functions] of the Langevin equation [0D]:

$$m\frac{\partial^2 x}{\partial t^2} = -\lambda\frac{\partial x}{\partial t} + \eta(t) \qquad \langle\eta(t)\eta(t')\rangle = 2\lambda T\delta(t-t')$$

●●●●●

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
      <dimension name="xbin" lattice="&NptsBin;" domain="(-&Xmax;,&Xmax;)" />
      <dimension name="vbin" lattice="&NptsBin;" domain="(-&Vmax;,&Vmax;)" />
  </transverse_dimensions>
</geometry>
```

Dimensions for sampling only

●●●●●

```
<vector name="variables" type="real" dimensions="">
  <components> pos  vel </components>
  <initialisation>
    <![CDATA[
      pos = 0.0;
      vel = 0.0;
    ]]>
  </initialisation>
</vector>
```

New: tell vectors in which dimensions they live (defaults to ALL dimensions)

hacking, see last section

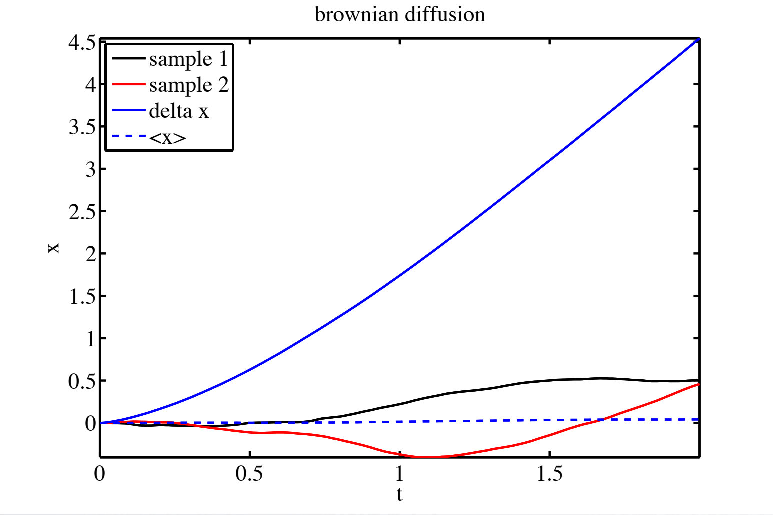
```
<group>
  <sampling  basis="" initial_sample="yes">
    <moments>position velocity</moments>
    <dependencies>variables</dependencies>
    <![CDATA[
      position = pos;
      velocity = vel;
    ]]>
  </sampling>
</group>
```

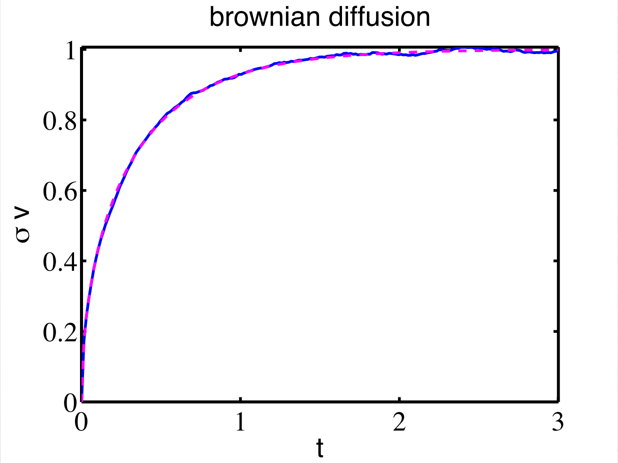
```
<group>
  <sampling  basis="xbin"  initial_sample="yes">
    <moments> pos_distribution </moments>
    <dependencies>variables</dependencies>
    <![CDATA[
     if(_index_xbin==0 && pos < (xbin+dxbin_halves))
       pos_distribution +=1.0;
     if( pos > (xbin-dxbin_halves) && pos < (xbin+dxbin_halves) )
       pos_distribution +=1.0;
     if(_index_xbin==_lattice_xbin-1 && pos >  (xbin-dxbin_halves) )
       pos_distribution +=1.0;
    ]]>
  </sampling>
</group>
```

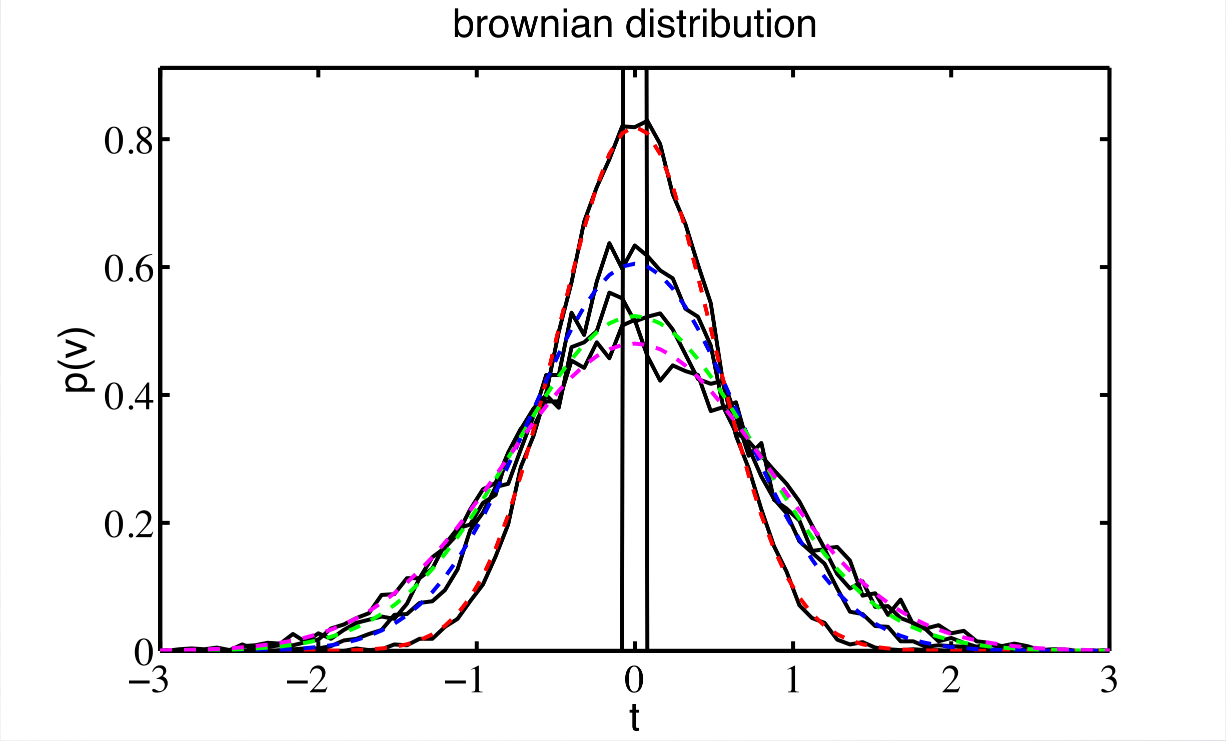
STOCHASTIC DE

- Langevin equation for brownian motion:

$$m\frac{\partial^2 x}{\partial t^2} = -\lambda\frac{\partial x}{\partial t} + \eta(t) \qquad \langle \eta(t)\eta(t')\rangle = 2\lambda T\delta(t-t')$$







COMMAND LINE PARAMETERS

see: GPE_1D_commandline_course.xmds

```
<features>
  <benchmark />
  <auto_vectorise />
  <fftw />
  <globals>
    <![CDATA[
    const double hbar = 1.05457266e-34;
    double omega = 10.0*(2.0*M_PI);           // to be modified by command line parameters
    const double omega_perp = 200.0*(2.0*M_PI);
    const double x0 = 0.0e-5;

    // Rb 87
    const double mass = 1.4432e-25;
    const double as = 5.5e-9;

    //dervied quantities
    const double Natoms = 100.0;

    const double U = 4.0*M_PI*hbar*hbar*as/mass;
    const double sigma_perp = sqrt(hbar/mass/omega_perp);
    const double U1d = U/(2.0*M_PI*sigma_perp*sigma_perp);

    double normfact = 0.0;    // get set after command line parameters are known
    double sigma = 0.0;
    ]]>
  </globals>
  <arguments>
     <argument name="trap_scale"  type="real" default_value="1.0"/>
     <argument name="width_scale" type="real" default_value="1.0"/>
     <![CDATA[
        omega *= sqrt(trap_scale);
        sigma = width_scale*sqrt(hbar/mass/omega);
        normfact = pow(M_PI*sigma*sigma,-0.25);
      ]]>
     </arguments>
</features>
```

Variables affected by command line parameters must be defined modifyable

Globals block evaluated BEFORE querying run time parameters

to pass on runtime

actions done AFTER querying run time parameters

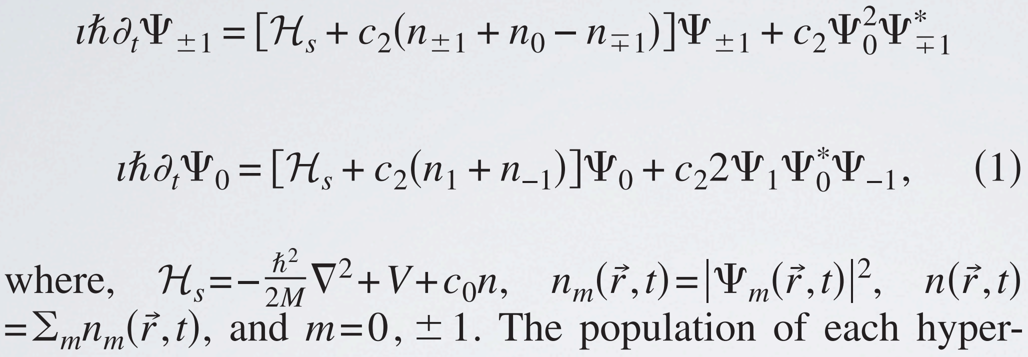
Execution: ./GPE_1D_commandline_course -t 15.0 -w 0.5

Execution: ./GPE_1D_commandline_course -trap_scale 15.0

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#wignerarguments

DISCRETE DIMENSIONS

- 1D Gross-Pitaevskii equation for **spinor BEC** (spin-1 atoms)



$$i\hbar\partial_t\Psi_{\pm1} = [\mathcal{H}_s + c_2(n_{\pm1} + n_0 - n_{\mp1})]\Psi_{\pm1} + c_2\Psi_0^2\Psi_{\mp1}^*$$

$$i\hbar\partial_t\Psi_0 = [\mathcal{H}_s + c_2(n_1 + n_{-1})]\Psi_0 + c_2 2\Psi_1\Psi_0^*\Psi_{-1}, \qquad (1)$$

where, $\mathcal{H}_s = -\frac{\hbar^2}{2M}\nabla^2 + V + c_0 n$, $n_m(\vec{r},t) = |\Psi_m(\vec{r},t)|^2$, $n(\vec{r},t) = \Sigma_m n_m(\vec{r},t)$, and $m = 0, \pm 1$. The population of each hyper-

taken from B. Julia-Diaz *et al.*
PRA **80** 043622 (2009).

- Wave function has subscript for spin state (mF=-1,0,1)

integer dimension for spin state

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>
```

XML comment

for constructions like:

$$\Psi_n = \sum_k C_{nk}\Psi_k$$

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#integerdimensionexample

DISCRETE DIMENSIONS

see: GPE_1D_spinor_course.xmds

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>
```

●●●●●

```
<vector name="wavefunction" initial_space="x n" type="complex">
  <components>psi</components>
    <initialisation>
      <![CDATA[
        double coeff = 0.0;

        if(n == 0)
           coeff = sqrt(0.1);
        if(n == 1)
           coeff = sqrt(0.8);
        if(n == 2)
           coeff = sqrt(0.1);

        psi = normfact*coeff*sqrt(Natoms)*exp(-0.5*x*x/sigma/sigma);
      ]]>
    </initialisation>
  </vector>
```

space and spin dependent Psi

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#wignerarguments

DISCRETE DIMENSIONS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>
```

……

```
<computed_vector name="auxiliary" dimensions="x" type="real">
  <components> totdens </components>
    <evaluation>
    <dependencies basis="x n"> wavefunction </dependencies>
    <![CDATA[
        totdens = mod2(psi);
    ]]>
  </evaluation>
</computed_vector>
```

again, excess dimensions are integrated (here summed) over

- calculation of: $n(\vec{r},t)=\Sigma_m n_m(\vec{r},t)$ $n_m(\vec{r},t)=|\Psi_m(\vec{r},t)|^2$

DISCRETE DIMENSIONS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>
```

matrix in spin space

```
<vector name="coupling" type="real" dimensions="n k">
  <components> F1 </components>
  <initialisation>
    <![CDATA[
      F1 = 0.0;

     // dpsi(-1)/dt
      if(n==0 && (k==0 || k==1))
        F1 = 1.0;
      if(n==0 && k ==2)
        F1 = -1.0;

     // dpsi(0)/dt
      if(n==1 && (k==0 || k==2))
        F1 = 1.0;

     // dpsi(+1)/dt
      if(n==2 && (k==1 || k==2))
        F1 = 1.0;
      if(n==2 && k ==0)
        F1 = -1.0;

    ]]>
  </initialisation>
</vector>
```

```
<computed_vector name="auxiliary2" dimensions="x n" type="real">
  <components> asymmdens </components>
    <evaluation>
    <dependencies basis="x n k"> wavefunction coupling</dependencies>
    <![CDATA[
        asymmdens = F1*mod2(psi( n=>k ));
    ]]>
  </evaluation>
</computed_vector>
```

again, excess dimensions are integrated (here summed) over, note use of alias

- calculation of:

$$\imath\hbar\partial_t\Psi_{\pm1} = \cdots (n_{\pm1}+n_0-n_{\mp1})$$

$$\imath\hbar\partial_t\Psi_0 = \cdots (n_1+n_{-1})$$

DISCRETE DIMENSIONS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>

<sequence>
  <integrate algorithm="ARK89" interval="4" tolerance="1e-8">
    <samples>200 200 200</samples>
    <operators>
      <operator kind="ip">
        <operator_names>L</operator_names>
        <![CDATA[
         L = -i*0.5*hbar*kx*kx/mass;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <dependencies>potentials auxiliary auxiliary2</dependencies>
      <![CDATA[
       complex conversion = 0.0;

       if(n == 0)
          conversion = conj(psi(n=>2))*psi(n=>1)*psi(n=>1);
       if(n == 1)
          conversion = 2.0*conj(psi)*psi(n=>n+1)*psi(n=>n-1);
       if(n == 2)
          conversion = conj(psi(n=>0))*psi(n=>1)*psi(n=>1);

       dpsi_dt =  L[psi] - i*( (U1ds*totdens + trap )*psi
                  + U1da*(asymmdens*psi  + conversion)   )/hbar;

       ]]>
    </operators>
  </integrate>
</sequence>
```

Final assembly

Non local addressing,
would have been clearer for this
example, but not for cases with
LARGE number of n

DISCRETE DIMENSIONS

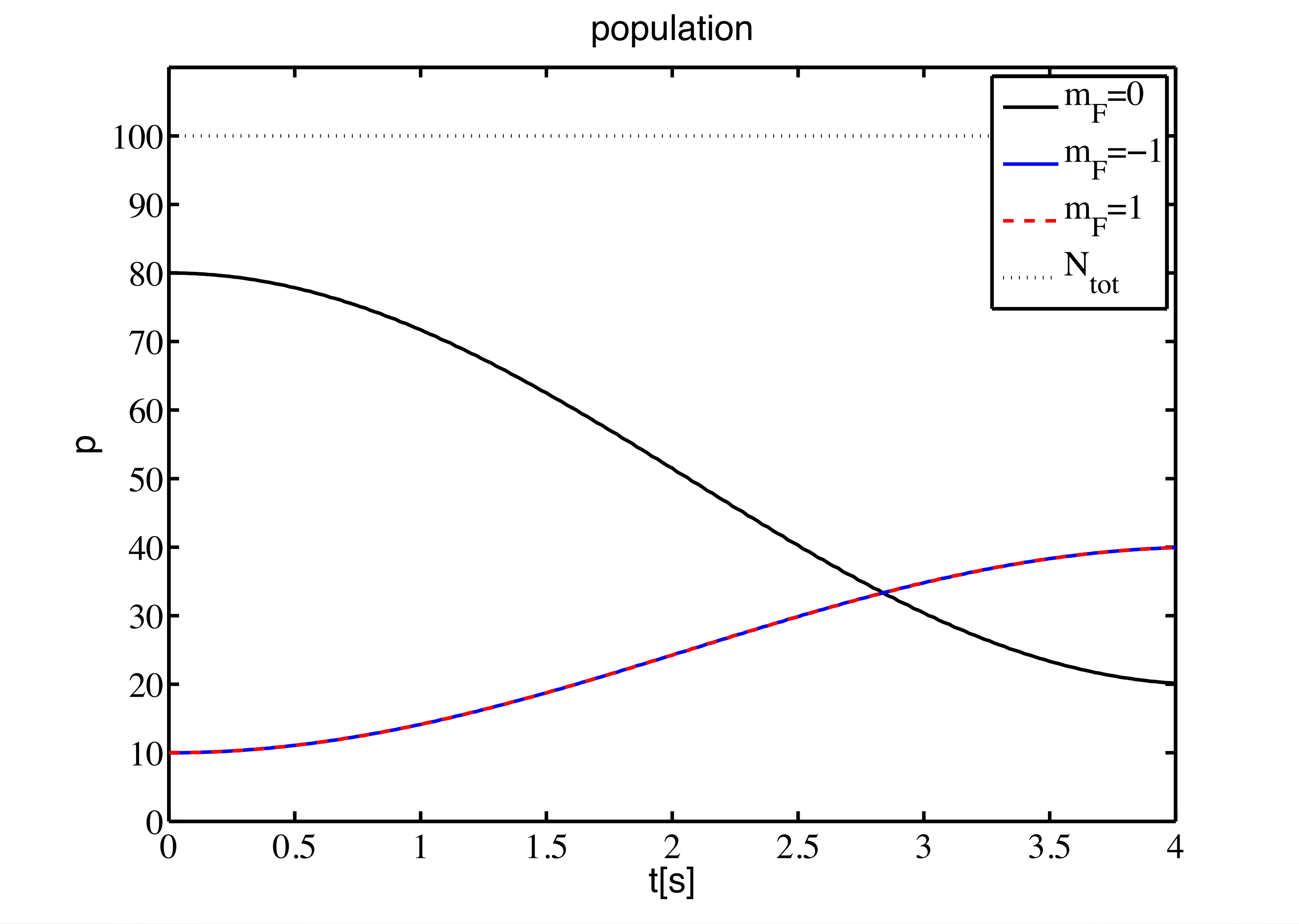
```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Npts;"  domain="(-&L;, &L;)" />
    <dimension name="n" type="integer" lattice="3"  domain="(0,2)" aliases="k"/>
    <!-- Assignment of components
           0: mF= -1
           1: mF=  0
           2: mF= +1  -->
   </transverse_dimensions>
</geometry>
```

Output now samples separately each spin component

```
<output format="hdf5">
  <group>
    <sampling basis="x(&Nsamples;) n" initial_sample="yes">
      <moments>density psire psiim  </moments>
      <dependencies>wavefunction </dependencies>
      <![CDATA[
        density = mod2(psi);
        psire = psi.Re();
        psiim = psi.Im();
      ]]>
    </sampling>
  </group>
```

Name	Size	Bytes	Class
density_1	201x64x3	308736	double

SPIN JOSEPHSON OSCILLATIONS



OSCILLATOR BASIS

- Harmonic oscillator Schroedinger equation, spectral solution

$$i\hbar\frac{d\psi}{dt} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right]\psi$$

- Eigenstates of TISE

$$E_n\phi_n = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right]\phi_n$$

- Spectral decomposition

$$\psi(x,t) = \sum_n c_n(t)\phi_n(x)$$

- TDSE in oscillator basis

$$i\hbar\frac{dc_n}{dt} = \hbar\omega(n + \frac{1}{2})c_n$$

OSCILLATOR BASIS

see: GPE_1D_hermites_course.xmds

- GPE in oscillator basis/ pos basis, split step

$$i\hbar\frac{d\psi}{dt} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2 + U|\psi|^2\right]\psi$$

$$i\hbar\frac{dc_n}{dt} = \hbar\omega(n+\frac{1}{2})c_n$$

$$U|\psi(x)|^2\psi(x)$$

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Nmodes;"
    length_scale="sqrt(hbar/(mass*omega))" transform="hermite-gauss" />
  </transverse_dimensions>
</geometry>
```

we explicitly give transform tag,
would default to "fourier"

●●●●●

```
<features>
  <benchmark />
  <auto_vectorise />
  <validation kind="run-time" />
```

Length scale: to get to
dimensionless hermites

Need this to use variables in
definition of length scale

see also http://xmds2.readthedocs.org/en/latest/worked_examples.html#hermitegaussgroundstatebec

OSCILLATOR BASIS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Nmodes;"
    length_scale="sqrt(hbar/(mass*omega))" transform="hermite-gauss" />
  </transverse_dimensions>
</geometry>
```

……

```
<vector name="wavefunction" initial_space="x" type="complex">
  <components>phi</components>
  <initialisation>
    <![CDATA[
       const double delx = x - x0;
       phi = normfact*sqrt(Natoms)*exp(-0.5*delx*delx/sigma/sigma);
    ]]>
  </initialisation>
</vector>
```

Now we can initialise in the energy basis. These two are equivalent for x0=0.

```
<vector name="wavefunction" initial_space="nx" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
       psi = 0.0;
       if(nx==0)
       psi = sqrt(Natoms);
    ]]>
  </initialisation>
</vector>
```

OSCILLATOR BASIS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="&Nmodes;"
    length_scale="sqrt(hbar/(mass*omega))" transform="hermite-gauss" />
  </transverse_dimensions>
</geometry>
```

●●●●●

```
<sequence>
  <integrate algorithm="ARK89" interval="0.4" tolerance="1e-8">
    <samples>200 200 200 200</samples>
    <operators>
      <operator kind="ip" constant="yes">
        <operator_names>L</operator_names>
        <![CDATA[
         L = -i*(nx + 0.5)*omega;
        ]]>
      </operator>
      <integration_vectors>wavefunction</integration_vectors>
      <![CDATA[
       double dens=psi.Re()*psi.Re() + psi.Im()*psi.Im();

       dpsi_dt =  L[psi] - i*U1d*dens*psi/hbar;

       ]]>
    </operators>
  </integrate>
</sequence>
```

Transform for application of IP operator is hermite-gauss

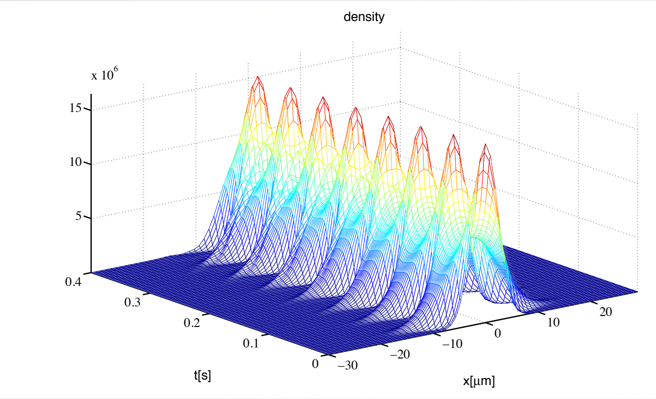
Nonlinear term evaluated in pos-space, in energy space would be nasty triple sum

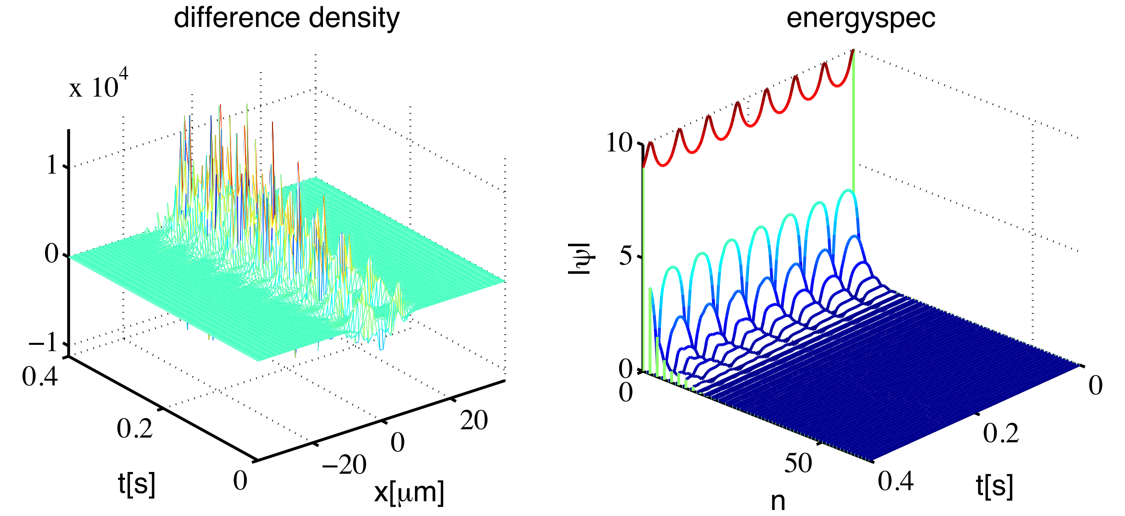
BASIS CHANGE

```
  <group>
    <sampling basis="nx(&Nmodes;)" initial_sample="yes">
      <moments>energyspec</moments>
      <dependencies>wavefunction</dependencies>
      <![CDATA[
        energyspec = mod2(psi);
      ]]>
   </sampling>
</group>
```

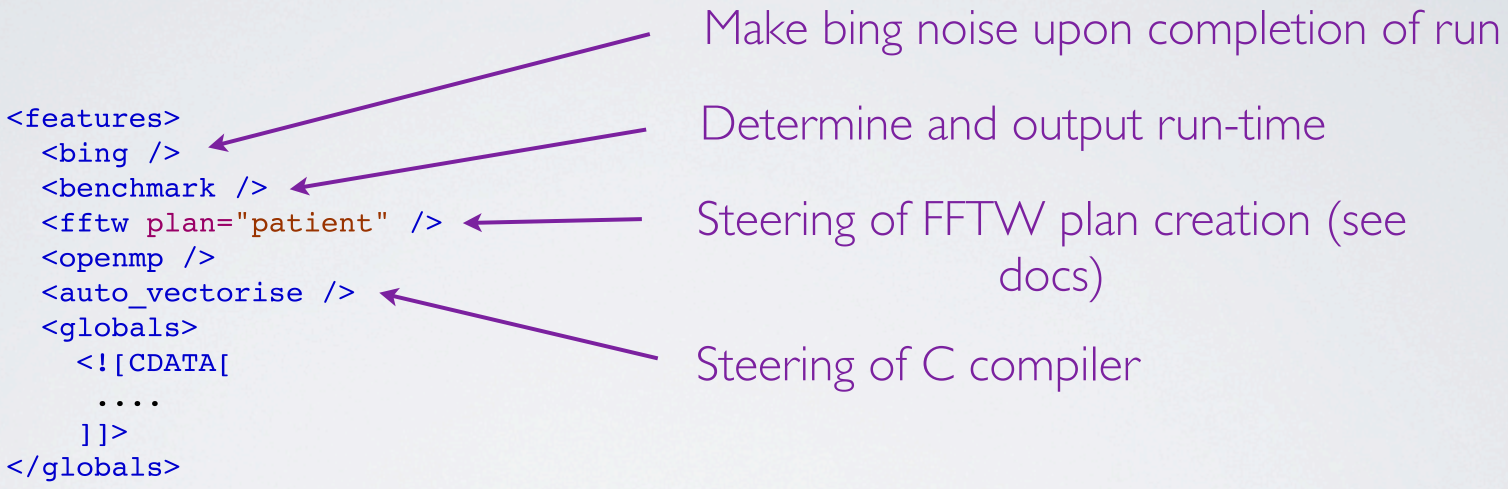
- Can sample in oscillator basis

- Compare breathing in oscillator and position basises





ASSORTED FURTHER TAGS



```
<features>
  <bing />
  <benchmark />
  <fftw plan="patient" />
  <openmp />
  <auto_vectorise />
  <globals>
    <![CDATA[
     ....
    ]]>
</globals>
```

Make bing noise upon completion of run

Determine and output run-time

Steering of FFTW plan creation (see docs)

Steering of C compiler

<diagnostics /> <!-- This will make sure that all nonlocal accesses of dimensions are safe -->

ASSORTED WARNINGS

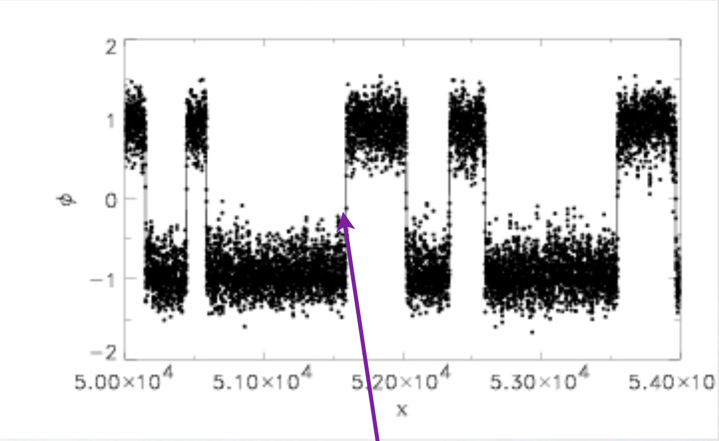
- If a tag has a non-existent name, it is just ignored. If in doubt, verify C code for existence of functionality.
- Fourier transforms have non-standard phases, see doc: http://xmds2.readthedocs.org/en/latest/advanced_topics.html#convolutions
- ...

EXERCISE TWO

- Kink bearing phi^4 classical field theory with noise
- taken from: S. Habib and G. Lythe, Phys. Rev. Lett. **84** 1070 (2000)
  http://www1.maths.leeds.ac.uk/~grant/research.html
- Equation of motion

$$\partial^2_{tt}\phi = \partial^2_{xx}\phi + \phi(1 - \phi^2) - \eta\partial_t\phi + \xi(x,t)$$

$$\langle \xi(x,t)\xi(x',t')\rangle = 2\eta\beta^{-1}\delta(x - x')\delta(t - t')$$



Kink solitons

- Simulation parameters:

Eta = 1, beta=7, Npts =256, Xmax=100, Tmax = 5e4.

XMDS HACKS

```
<geometry>
  <propagation_dimension> t </propagation_dimension>
  <transverse_dimensions>
    <dimension name="x" lattice="4096"  domain="(-4.0, 4.0)" />
  </transverse_dimensions>
</geometry>
```

- Useful internal variables:

_max_x=4,

_min_x=-4,

_lattice_x=4096

```
</features>

<vector name="wavefunction" initial_space="x" type="complex">
  <components>psi</components>
  <initialisation>
    <![CDATA[
      psi = N/cosh(x);
    ]]>
  </initialisation>
</vector>
```

```
<group>
  <sampling basis="x(512)" initial_sample="yes">
    <moments>density</moments>
    <dependencies>wavefunction</dependencies>
    <![CDATA[
      density = mod2(psi);
```

_mg0_output_lattice_t

_mg0_output_index_t

_index_x

_x_wavefunction_ncomponents

_active_x_wavefunction[_lattice_x]

- If you know SOME C, don't hesitate to look at the written .cc file. Search for your xmds CDATA text....

XMDS HACKS

see: GPE_1D_hacks_course.xmds

- Knowing the internal structure of the .cc code, we can add most things we would want to our XMDS code:

```
  <features>
    <benchmark />
    <auto_vectorise />
    <fftw />
    <globals>
      <![CDATA[
      #include "gsl_sf_hyperg.h"

      ●●●●●

     //%%%%%%%%%%%%%%%
     // FUNCTION LIBRARY

     void calculate_useless_hypergeometric_functions(){

         gsl_sf_result result;

         int status=gsl_sf_hyperg_1F1_e(t,1.5,0.3,&result);

         hypergeos[counter] = result.val;
         counter++;

     }
    //%%%%%%%%%

    void display_useless_hypergeometric_functions(){

        for(int nn=0;nn<_mg0_output_lattice_t;nn++)
          printf("Hyper[%i] = %e\n",nn,hypergeos[nn]);

    }

    ]]>
  </globals>
</features>
```

Bind in extra libraries

↓

```
xmds2 --configure --include-path $GSL_HOME/include/gsl --lib-path $GSL_HOME/lib
```

```
xmds2 GPE_1D_hacks_course.xmds -g
```

debug switch, outputs compiler statement

XMDS HACKS

- Knowing the internal structure of the .cc code, we can add most things we would want to our XMDS code:

```
<sequence>
  <integrate algorithm="ARK89" interval="0.4" tolerance="1e-8">

   ●●●●●

   </integrate>
   <filter>
      <![CDATA[
          display_useless_hypergeometric_functions();
          write_extra_output();
       ]]>
  </filter>
 </sequence>
```

Write non-standard sampling at end

```
 ●●●●●

 <group>
   <sampling basis="x(&Nsamples;)" initial_sample="yes">
     <moments>density psire psiim </moments>
     <dependencies>wavefunction </dependencies>
     <![CDATA[
       density = mod2(psi);
       psire = psi.Re();
       psiim = psi.Im();

       if(_index_x==0)
          calculate_useless_hypergeometric_functions();
     ]]>
   </sampling>
 </group>
```

Sample whenever we sample _mg0

XMDS HACKS

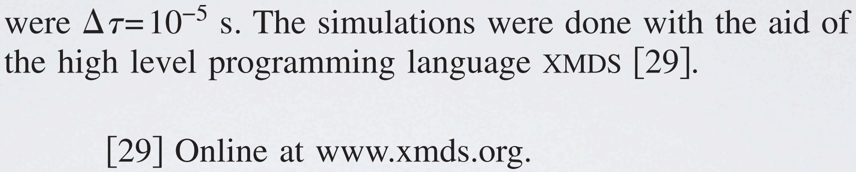
- Knowing the internal structure of the .cc code, we can add most things we would want to our XMDS code:

```
<globals>
  <![CDATA[

   ●●●●●

   //%%%%%%%%%%%%%%%
   //% output
   unsigned long counter=0;
   double hypergeos[_mg0_output_lattice_t];

   const char *outfilename="GPE_1D_hacks_course_additional_output.data";
   fstream outfile;

   ●●●●●

   //%%%%%%%%%%

   void write_extra_output(){
       printf("Writing additional output to: %s \n",outfilename);
       outfile.open(outfilename,ios::out|ios::binary);
       outfile.write((char*)hypergeos,sizeof(double)*_mg0_output_lattice_t);

       if(outfile.bad()){
          printf("Error writing MGs to file, wrote %i bytes.\n",outfile.gcount());
          exit(42);
       }

       outfile.close();

   }

  ●●●●●
    ]]>
  </globals>
```

Perform file I/O
as in usual C

ACKNOWLEDGE XMDS

- If you publish something done mainly with XMDS, please place a reference:



were $\Delta\tau = 10^{-5}$ s. The simulations were done with the aid of the high level programming language XMDS [29].

[29] Online at www.xmds.org.

- Maybe at some point submit your code as example to the XMDS webpage

IMPROVE XMDS

- If you need a new feature (basis, sampling etc.) consider adding it to XMDS itself, sign up at:

http://sourceforge.net/projects/xmds/

XMDS2 BROUGHT TO YOU BY:

Graham Dennis

Joe Hope

Mattias Johnsson

Michael Hush

BASED ON XMDS1 BY:

Greg Collecut

Joe Hope

Clinton Roy

Paul Cochrane

Michael East

et al.

Thanks for your attention