PAUL SCHERRER INSTITUT

PSI

Matthias Frey :: Paul Scherrer Institut

Cyclotron Simulations with OPAL

14 September 2020 :: OPAL Introduction

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Outline

General Information

How to run OPAL?

Setup of Input File for Cyclotron Simulations

Units

OPAL Output Files

OPAL-Optimizer

OPAL-Sampler

Data Postprocessing & Visualization with pyOPALTools

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General Information

- **Wiki:**
  https://gitlab.psi.ch/OPAL/src/-/wikis/home
  - Compile instructions
  - Available binaries for Linux and macOS
  - Examples
  - OPAL Mailing list subscription at
    https://psilists.ethz.ch/sympa/subscribe/opal
- **Source Code:**
  `git clone https://gitlab.psi.ch/OPAL/src.git`
- **Manual:**
  http://amas.web.psi.ch/opal/Documentation/master/index.html

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Running OPAL on your Laptop and on HPC cluster

Assuming the OPAL executable is part of your `$PATH` environment variable!

- **Single Core:** `$ opal [inputfile.in]`

```
Ippl> CommMPI: Parent process waiting for children ...
Ippl> CommMPI: Initialization complete.
>                 ____   _____        ___
>                / __ \|  __ \ /\    | |
>               | |  | | |__) /  \   | |
>               | |  | |  ___/ /\ \  | |
>               | |__| | |  / ____ \| |____
>                \____/|_| /_/    \_\______|
OPAL>
OPAL> This is OPAL (Object Oriented Parallel Accelerator Library) Version 2.4.0
OPAL>              git rev. 1fd20f79e78e1e3dbbdd21d12416b52d688120c1
OPAL>
OPAL>
OPAL>                        (c) PSI, http://amas.web.psi.ch
OPAL>
...
```

Running OPAL on your Laptop and on HPC cluster

Assuming the OPAL executable is part of your `$PATH` environment variable!

- **Multiple Cores:** `$ mpirun -np [number of cores] opal [inputfile.in]`

```
Ippl> CommMPI: Parent process waiting for children ...
Ippl> CommMPI: Started job 1 on host 'R2-D2'.
Ippl> CommMPI: Started job 2 on host 'R2-D2'.
Ippl> CommMPI: Started job 3 on host 'R2-D2'.
Ippl> CommMPI: Child 2 ready.
Ippl> CommMPI: Child 1 ready.
Ippl> CommMPI: Child 3 ready.
Ippl> CommMPI: Initialization complete.
{0}>                 ____  _____        ___
{0}>                / __ \|  __ \ /\    | |
{0}>               | |  | | |__) /  \   | |
{0}>               | |  | |  ___/ /\ \  | |
{0}>               | |__| | |  / ____ \| |____
{0}>                \____/|_| /_/    \_\______|
OPAL{0}>
OPAL{0}> This is OPAL (Object Oriented Parallel Accelerator Library) Version 2.1.0
OPAL{0}>              git rev. 88400b8ffdcba529ace97bd6f40d16c55d9e4ca8
OPAL{0}>
OPAL{0}>
OPAL{0}>                          (c) PSI, http://amas.web.psi.ch
OPAL{0}>
...
```

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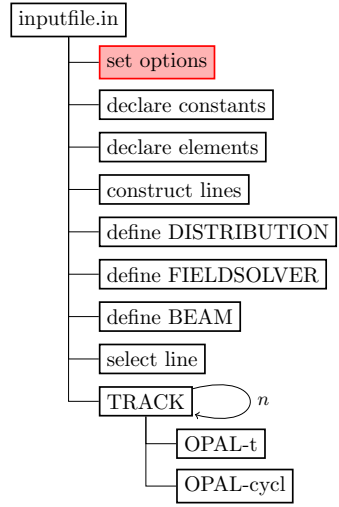
Setup of Input File – Cyclotron Example

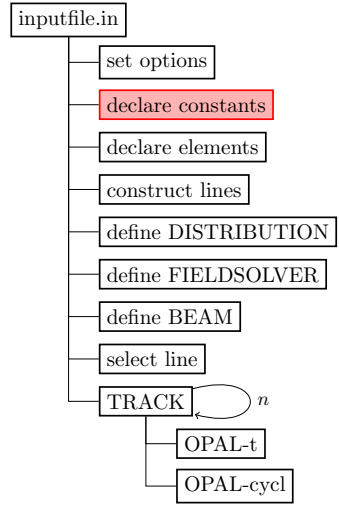
```
Option, PSDUMPFREQ      = 10;     // H5 phase space dump
Option, SPTDUMPFREQ     = 10;     // single particle dump
Option, PSDUMPEACHTURN  = false;  // H5 turn dump
Option, STATDUMPFREQ    = 1;      // statistics dump
Option, VERSION=20400;            // OPAL 2.4.0
...
```

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#sec.control.option



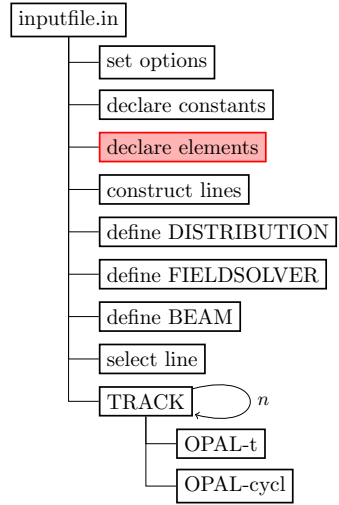
Setup of Input File – Cyclotron Example

```
REAL Ekin    = 0.072;                // [GeV]
REAL gamma   = (Ekin+PMASS)/PMASS;
REAL beta    = sqrt(1-(1/gamma^2));
REAL gambet  = gamma*beta;
REAL P0      = gamma*beta*PMASS;

VALUE,{gamma,beta,gammabeta,Ekin}; // print values
```



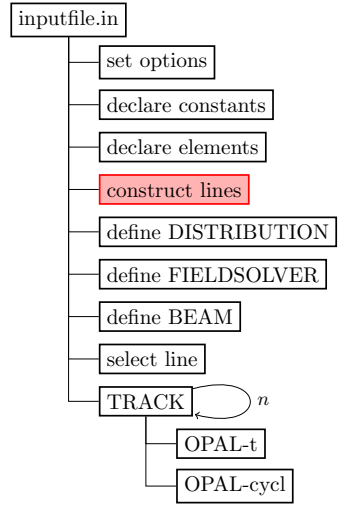
Setup of Input File – Cyclotron Example

```
ring: CYCLOTRON, TYPE="RING", CYHARMON=6, PHIINIT=0.0,
                 PRINIT=-0.000174, RINIT=2130.0,
                 SYMMETRY=8.0, RFFREQ=frequency,
                 FMAPFN="s03av.nar";

rf0: RFCAVITY, VOLT=volt1st, FMAPFN="Cav1.dat",
               TYPE="SINGLEGAP", FREQ=frequency,
               RMIN = 1900.0, RMAX = 4500.0,
               ANGLE=35.0,  PDIS = 416.0,
               GAPWIDTH = 220.0, PHI0=phi01;

rf1: RFCAVITY, ...;
rf2: RFCAVITY, ...;
rf3: RFCAVITY, ...;
rf4: RFCAVITY, ...;
```



Setup of Input File – Cyclotron Example

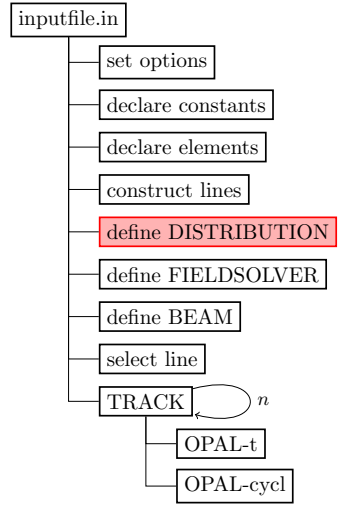
```
l1: LINE = (ring, rf0, rf1, rf2, rf3, rf4);
```



Setup of Input File – Cyclotron Example

```
Dist1: DISTRIBUTION, TYPE=GAUSS, SIGMAX  = 2.0e-03,
                                 SIGMAPX = 1.0e-7,
                                 CORRX   = 0.0,
                                 SIGMAY  = 2.0e-03,
                                 SIGMAPY = 1.0e-7,
                                 CORRY   = 0.0,
                                 SIGMAT  = 2.0e-03,
                                 SIGMAPT = 3.394e-4,
                                 CORRT   = 0.0;
```

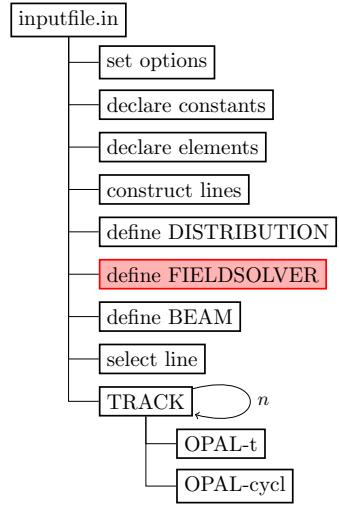
Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.distribution



Setup of Input File – Cyclotron Example

```
Fs1: FIELDSOLVER, FSTYPE = FFT,    // Fourier solver
                  MX     = 32,     // no. grid points
                  MY     = 32,
                  MT     = 16,
                  PARFFTX = true, // parallelize?
                  PARFFTY = true,
                  PARFFTT = true,
                  BCFFTX  = open, // boundary condition
                  BCFFTY  = open,
                  BCFFTZ  = open;
```

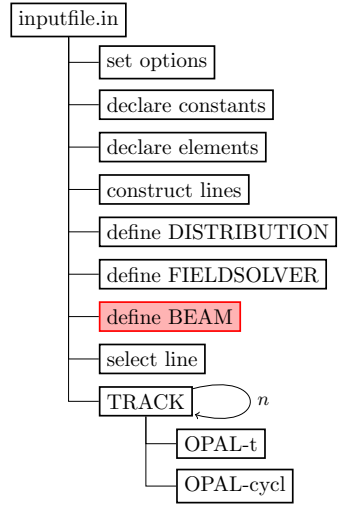
Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#sec.fieldsolvers.fieldsolvercmd



Setup of Input File – Cyclotron Example

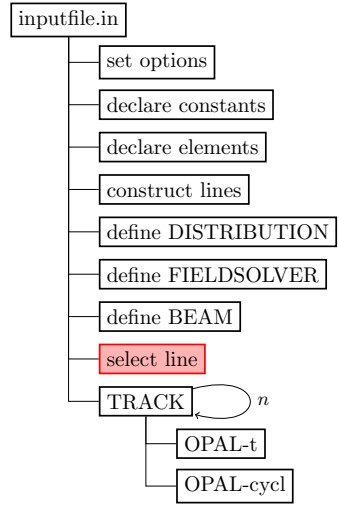
```
beam1: BEAM, PARTICLE = PROTON,
             PC       = P0,
             NPART    = 1e5,
             BCURRENT = 1.0E-3,
             CHARGE   = 1.0,
             BFREQ    = frequency;
```

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.beam-command



Setup of Input File – Cyclotron Example

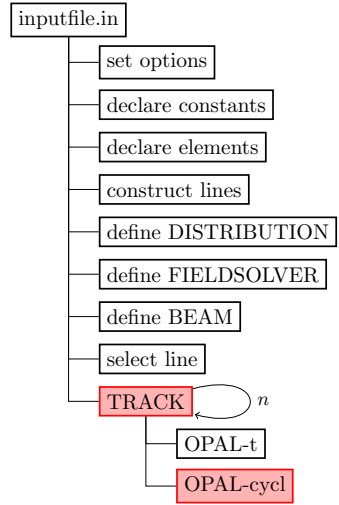
```
SELECT, LINE = l1;
```



Setup of Input File – Cyclotron Example

```
TRACK, LINE            = l1,
       BEAM            = beam1,
       MAXSTEPS        = nstep*turns,
       STEPSPERTURN    = nstep,
       TIMEINTEGRATOR  = "RK-4";

RUN, METHOD        = "CYCLOTRON-T",
     BEAM          = beam1,
     FIELDSOLVER   = Fs1,
     DISTRIBUTION  = Dist1;

ENDTRACK;

STOP;
```

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.track



Input File Example – Part I of IV

```
Option, ECHO=FALSE;
Option, PSDUMPFREQ=60;
Option, SPTDUMPFREQ = 10;
Option, PSDUMPEACHTURN=false;
Option, REPARTFREQ=20;
Option, ECHO=FALSE;
Option, STATDUMPFREQ=1;
Option, CZERO=FALSE;
Option, TELL=TRUE;
Option, VERSION=20400;

Title,string="OPAL-cycl: the first 10 turns in PSI 590MeV Ring";

REAL Edes=.072;
REAL gamma=(Edes+PMASS)/PMASS;
REAL beta=sqrt(1-(1/gamma^2));
REAL gambet=gamma*beta;
REAL P0 = gamma*beta*PMASS;
REAL brho = (PMASS*1.0e9*gambet) / CLIGHT;

//value,{gamma,brho,Edes,beta,gambet};
```

Input File Example – Part II of IV

```
REAL phi01=139.4281;
REAL phi02=phi01+180.0;
REAL phi04=phi01;
REAL phi05=phi01+180.0;
REAL phi03=phi01+10.0;

REAL volt1st=0.9;
REAL volt3rd=0.9*4.0*0.112;

REAL turns = 10;
REAL nstep=360;

REAL frequency=50.650;
REAL frequency3=3.0*frequency;

ring: Cyclotron, TYPE="RING", CYHARMON=6, PHIINIT=0.0,
    PRINIT=-0.000174, RINIT=2130.0, SYMMETRY=8.0, RFFREQ=frequency,
    FMAPFN="s03av.nar";

rf0: RFCavity, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE="SINGLEGAP",
    FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=35.0,  PDIS = 416.0,
    GAPWIDTH = 220.0, PHI0=phi01;
```

Input File Example – Part III of IV

```
rf1: RFCavity, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE="SINGLEGAP",
    FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=125.0, PDIS = 416.0,
    GAPWIDTH = 220.0, PHI0=phi02;

rf2: RFCavity, VOLT=volt3rd, FMAPFN="Cav3.dat", TYPE="SINGLEGAP",
    FREQ=frequency3,RMIN = 1900.0, RMAX = 4500.0, ANGLE=170.0, PDIS = 452.0,
    GAPWIDTH = 250.0, PHI0=phi03;

rf3: RFCavity, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE="SINGLEGAP",
    FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=215.0, PDIS = 416.0,
    GAPWIDTH = 220.0, PHI0=phi04;

rf4: RFCavity, VOLT=volt1st, FMAPFN="Cav1.dat", TYPE="SINGLEGAP",
    FREQ=frequency, RMIN = 1900.0, RMAX = 4500.0, ANGLE=305.0, PDIS = 416.0,
    GAPWIDTH = 220.0, PHI0=phi05;

l1:   Line = (ring,rf0,rf1,rf2,rf3,rf4);
```

Input File Example – Part IV of IV

```
Dist1:DISTRIBUTION, TYPE=gauss,
    sigmax = 2.0e-03,
    sigmapx = 1.0e-7,
    corrx = 0.0,
    sigmay = 2.0e-03,
    sigmapy = 1.0e-7,
    corry = 0.0,
    sigmat = 2.0e-03,
    sigmapt = 3.394e-4,
    corrt=0.0;

Fs1:FIELDSOLVER, FSTYPE=FFT, MX=32, MY=32, MT=16,
    PARFFTX=true, PARFFTY=true, PARFFTT=true,
    BCFFTX=open, BCFFTY=open, BCFFTT=open, BBOXINCR=2;

beam1: BEAM, PARTICLE=PROTON, pc=P0, NPART=1e5, BCURRENT=1.0E-3, CHARGE=1.0, BFREQ= frequency;

Select, Line=l1;

TRACK,LINE=l1, BEAM=beam1, MAXSTEPS=nstep*turns, STEPSPERTURN=nstep,TIMEINTEGRATOR="RK-4";
 run, method = "CYCLOTRON-T", beam=beam1, fieldsolver=Fs1, distribution=Dist1;
endtrack;

Stop;
```

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OPAL Units

A consistent set of units is still work in progress

Quantity	Dimension
Length	m (metres) & mm (OPAL-cycl)
Angle	rad (radians) & deg (OPAL-cycl)
Quadrupole coefficient	Tm^{-1}
Multipole coefficient, 2n poles	Tm^{-n+1}
Electric voltage	MV (Megavolts)
Electric field strength	MV/m
Frequency	MHz (Megahertz)
Particle energy	MeV or eV
Particle mass	$\mathrm{MeV/c}^2$
Particle momentum	$\beta\gamma$ or eV
Beam current	A (Amperes)
Particle charge	e (elementary charges)
Impedances	MΩ (Megohms)
Emittances[1]	m rad
RF power	MW (Megawatts)

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#sec.conventions.units

[1] (normalized and geometric)

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OPAL Output Files

Running OPAL with the input file `inputfile.in` generates following output files:

- `inputfile.h5`
  File storing full particle phase space data; also used for restarts
- `inputfile.stat`
  Bunch statistics stored in SDDS format
- `inputfile-trackOrbit.dat`
  Orbit of reference particle and particle with small deviation from reference orbit
- `inputfile-afterEachTurn.dat`
  Phase space data in global cylindrical coordinates after each turn; single particle mode only
- `inputfile-Angle{0,1,2}.dat`
  Phase space data at azimuth $\theta = 0, \frac{\pi}{8}, \frac{\pi}{4}$ in global cylindrical coordinates; single particle mode only
- `inputfile.lbal`
  Load-balancing of particles among MPI ranks

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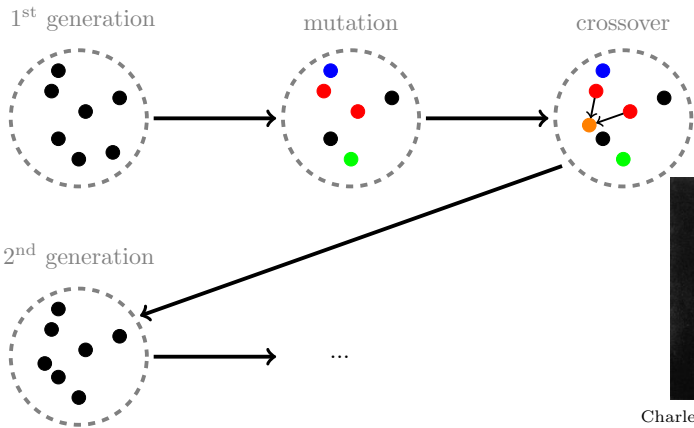
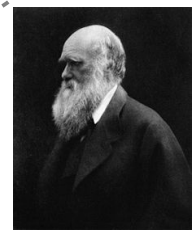
Optimization with Multiobjective Genetic Algorithm[2]





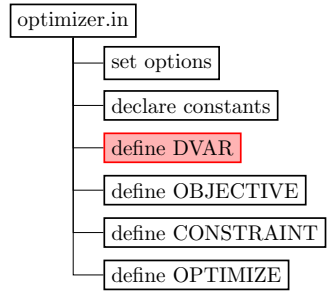
Charles Darwin (Wikipedia)

[2] Y. Ineichen, Toward massively parallel multi-objective optimisation with application to particle accelerators. Diss. ETH No. 21114 (2013)

Optimization with Multiobjective Genetic Algorithm[2]

```
dv1: DVAR, VARIABLE="varname",   // variable name
           LOWERBOUND=0.1,       // lower bound
           UPPERBOUND=0.2;       // upper bound
```

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.optimiser



[2] Y. Ineichen, Toward massively parallel multi-objective optimisation with application to particle accelerators. Diss. ETH No. 21114 (2013)

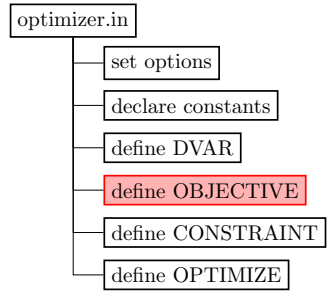
Optimization with Multiobjective Genetic Algorithm[2]

```
obj1: OBJECTIVE, EXPR="expression";
```

Example:

```
drmsx: OBJECTIVE,
       EXPR="fabs(statVariableAt('rms_x', 2.0))";
```

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.optimiser



[2] Y. Ineichen, Toward massively parallel multi-objective optimisation with application to particle accelerators. Diss. ETH No. 21114 (2013)

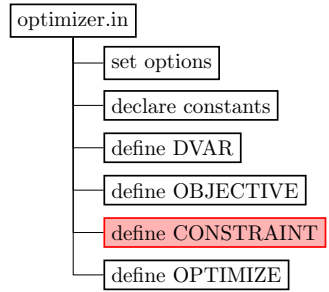
Optimization with Multiobjective Genetic Algorithm[2]

```
con1: CONSTRAINT, EXPR="expression";
```

Example:

```
crmsx: CONSTRAINT,
       EXPR="statVariableAt('rms_x', 1.0) < 0.003";
```

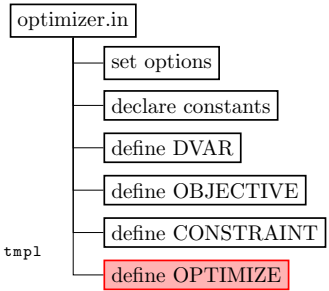
Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.optimiser



[2] Y. Ineichen, Toward massively parallel multi-objective optimisation with application to particle accelerators. Diss. ETH No. 21114 (2013)

Optimization with Multiobjective Genetic Algorithm[2]

```
OPTIMIZE, INPUT="inputfile.tmpl",
          OBJECTIVES             = {obj1, obj2, ...},
          DVARS                  = {dv1, dv2, ...},
          INITIALPOPULATION      = 5,
          MAXGENERATIONS         = 10,
          NUM_IND_GEN            = 5,
          MUTATION_PROBABILITY   = 0.43,
          SIMBIN_CROSSOVER_NU    = 2.0,
          NUM_MASTERS            = 1,
          NUM_COWORKERS          = 2,
          SIMTMPDIR              = "simtmpdir", // simulation directory
          TEMPLATEDIR            = "template",  // directory of inputfile.tmpl
          FIELDMAPDIR            = "fieldmaps",
          OUTPUT                 = "outname",
          OUTDIR                 = "results",
          KEEP                   = {STAT, IN, H5};  // do not delete
```



Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.optimiser

[2] Y. Ineichen, Toward massively parallel multi-objective optimisation with application to particle accelerators. Diss. ETH No. 21114 (2013)

Template File vs. Input File

- A template file is like an input file.
- **But:** All design variables need to be defined in the template file.
- **Example:**

optimizer.in

```
dv1: DVAR, VARIABLE="bcurrent",  // beam current
           LOWERBOUND=0.001,     // [A]
           UPPERBOUND=0.002;     // [A]
```

inputfile.tmpl

```
beam1: BEAM, PARTICLE = PROTON,
             PC       = P0,
             NPART    = 1e5,
             BCURRENT = _bcurrent_,
             CHARGE   = 1.0,
             BFREQ    = frequency;
```

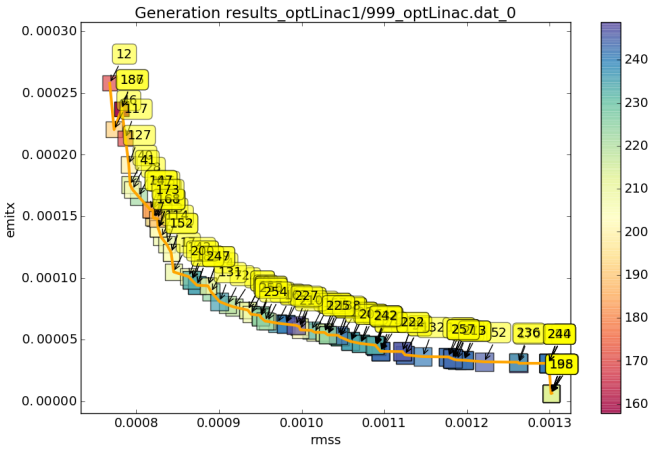
Optimizer Output

- A **JSON**[3] file **per generation**
- A **JSON** file with **pareto front** individuals


```
{
    "name": "opt-pilot",
    "OPAL version": "2.3.0",
    "git revision": "7f506bf9abbe51f800e5cc5c5d991712adbc59bb",
    "dvar-bounds": {
        "sigmax": "[ 0.002, 0.0022 ]"
    },
    "constraints": "",
    "population": {
        "1": {
            "obj": {
                "GOALFUN": "0.0019817400858543012"
            },
            "dvar": {
                "sigmax": "0.0020306983200833201"
            }
        },
...
```


[3] JavaScript Object Notation

Pareto Front?



(Taken from https://gitlab.psi.ch/OPAL/opt-pilot/wikis/optpilot-week)

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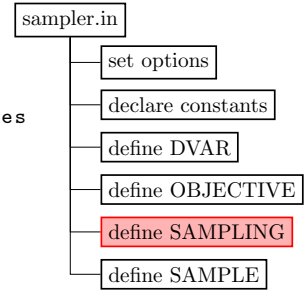
Sampler

```
sm1: SAMPLING, VARIABLE = "varname",
               TYPE     = "UNIFORM",
               SEED     = 42,
               N        = 100;        // number of samples
```

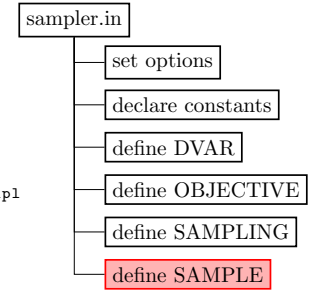
TYPE = FROMFILE, GAUSSIAN, ...

Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.sampler



Sampler

```
SAMPLE, RASTER                = false,
        INPUT                 = "inputfile.tmpl",
        SAMPLINGS             = {sm1, sm1, ...},
        DVARS                 = {dv1, dv2, ...},
        OBJECTIVES            = {obj1, obj2, ...},
        NUM_MASTERS           = 1,
        NUM_COWORKERS         = 2,
        SIMTMPDIR             = "simtmpdir", // simulation directory
        TEMPLATEDIR           = "template",  // directory of inputfile.tmpl
        FIELDMAPDIR           = "fieldmaps",
        OUTPUT                = "outname",
        OUTDIR                = "results",
        KEEP                  = {STAT, IN, H5};  // keep only
```



Manual:
http://amas.web.psi.ch/opal/Documentation/master/index.html#chp.sampler

Sampler Output

- A JSON file **per master**

```
{
    "name": "sampler",
    "OPAL version": "2.4.0",
    "git revision": "1fd20f79e78e1e3dbbdd21d12416b52d688120c1",
    "dvar-bounds": {
        "numparticles": "[ 4096, 8192 ]"
    },
    "samples": {
        "0": {
            "dvar": {
                "numparticles": "4096"
            },
            "obj": {
                "OBJ1": "0.00083601928199118259"
            }
        },
        "1": {
            "dvar": {
                "numparticles": "4551"
            },
            "obj": {
                "OBJ1": "0.00083433398855364176"
            }
        },
...
```

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Outline

General Information

How to run OPAL?

Setup of Input File for Cyclotron Simulations

Units

OPAL Output Files

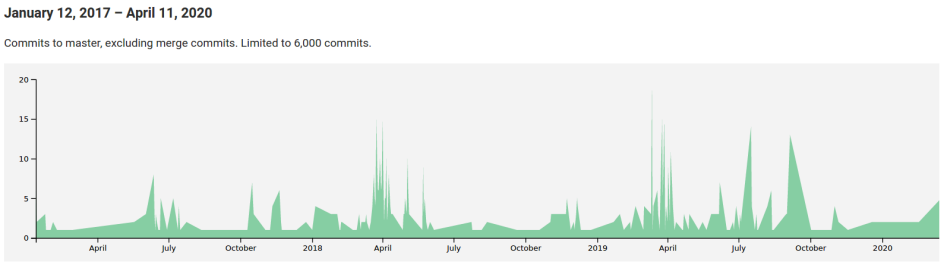
OPAL-Optimizer

OPAL-Sampler

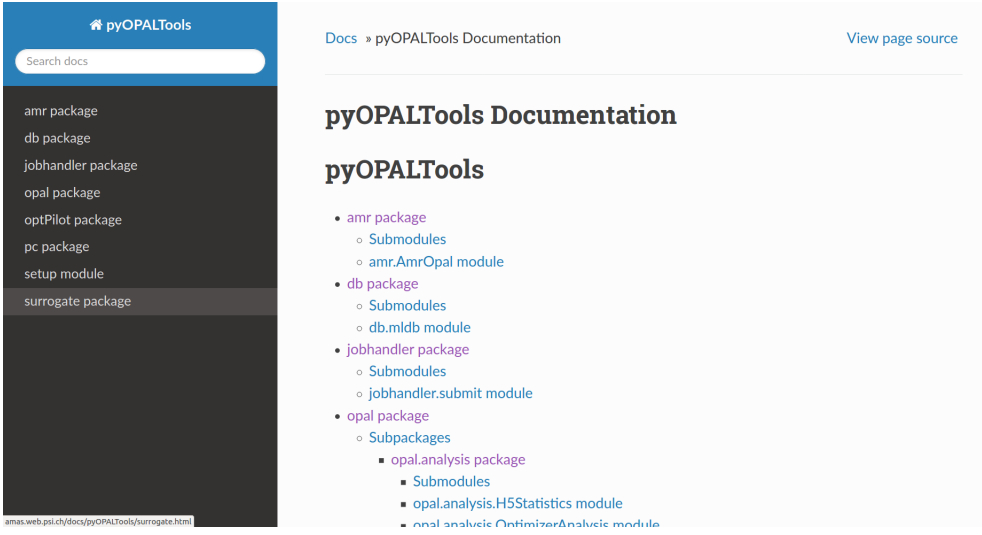
Data Postprocessing & Visualization with pyOPALTools

pyOPALTools – Repository on PSI GitLab

- Website: https://gitlab.psi.ch/OPAL/pyOPALTools
- Checkout: `git clone https://gitlab.psi.ch/OPAL/pyOPALTools.git`
  (developers: `git clone git@gitlab.psi.ch:OPAL/pyOPALTools.git`)
- Under development – contributors are welcome!



Sphinx Documentation – Link via Wiki of Repository



Data Loading

```
from opal import load_dataset, filetype

# load a specific file (here HDF5) using its file name
ds = load_dataset(directory='/path/to/files/',
                  fname='filename.h5')

# show summary of dataset
print(ds)

# load files using their file type (here HDF5)
dsets = load_dataset(directory='/path/to/files/',
                     ftype=filetype.H5)
```

Data Access

```
# obtain array of positions of macroparticles in x-direction at step 1
x_data  = ds.getData(var='x', step=1)

# unit of positions
x_unit  = ds.getUnit(var='x')

# variable name, mainly used as axis labels
x_label = ds.getLabel(var='x')
```

OPAL Package – Unified Interface to do Data Analysis

file type	format	description
AMR	HyperCLaw-V1.1[4]	particle phase space and AMR grid data
GRID	SDDS	AMR load balancing
HIST	ASCII	histogram of the radial positions of the particles at probe elements
H5	HDF5	particle phase space, used as a check point file
LBAL	SDDS	load balancing of macroparticles
LOSS	ASCII	phase space data of particles lost at elements (e.g., collimator, stripper)
MEM	SDDS	virtual memory consumption
OPTIMIZER	JSON	generation files and Pareto file of multiobjective genetic algorithm
OUTPUT	ASCII	OPAL standard output
PEAK	ASCII	peak values of the histogram generated by a radial probe
SAMPLER	JSON	all individual simulations of a sample run
SMB	SDDS	statistical measures of individual bunches of a neighboring bunch model
SOLVER	SDDS	AMR multigrid solver convergence information
STAT	SDDS	statistical measures of the bunch
TIMING	ASCII	runtime of individual code sections
TRACK_ORBIT	ASCII	single particle phase space data

[4] A file format of AMReX.

Data Plotting

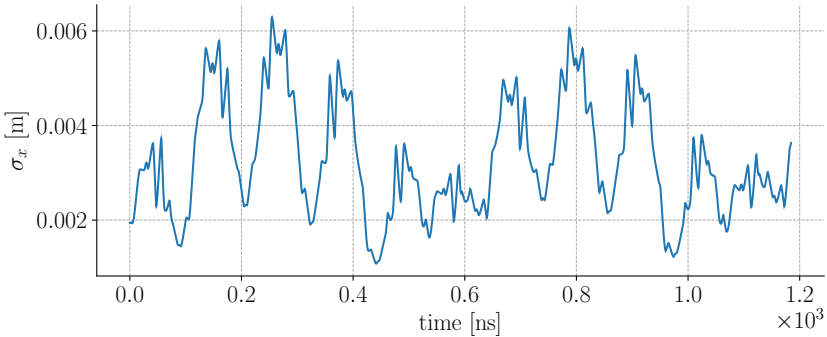
```
# set the plotting style
from opal.visualization.styles import load_style

load_style('jupyter') # 'default' or 'poster'

# load the dataset
from opal.opal import load_dataset
ds = load_dataset('.', fname='RingCyclotron.stat')

# create plot
import matplotlib.pyplot as plt
plt.figure(figsize=(9, 4))
plt = ds.plot_profile1D('time', 'rms_x', xsci=True)
plt.grid(linestyle='dashed')
plt.tight_layout()
plt.show()
```

OPAL Package – Unified Interface to do Data Analysis

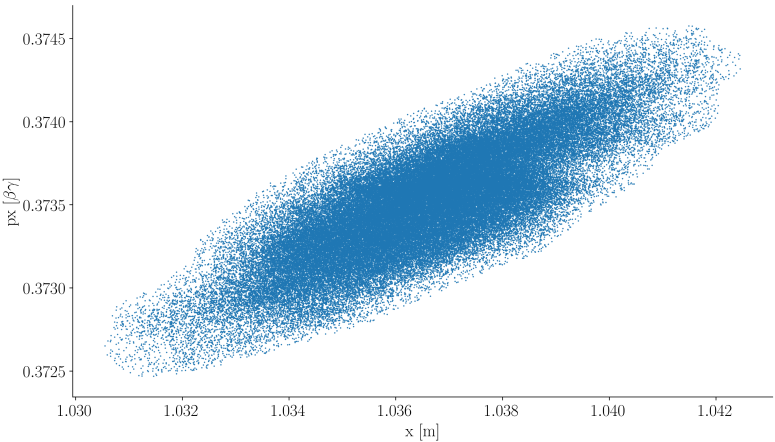


Data Plotting

```
# load the dataset
ds = load_dataset('.', fname='RingCyclotron.h5')

# create plot
plt = ds.plot_phase_space('x', 'px', step=5)
plt.show()
```

OPAL Package – Unified Interface to do Data Analysis

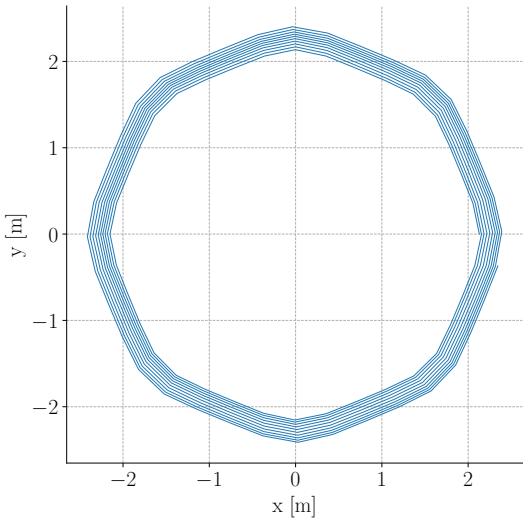


Data Plotting

```
# load the dataset
ds = load_dataset('.', fname='RingCyclotron-trackOrbit.dat')

# create plot
plt = ds.plot_orbits(linewidth=0.5)
plt.gca().set_aspect('equal')
plt.grid(linestyle='dashed')
plt.show()
```

OPAL Package – Unified Interface to do Data Analysis



Thanks to

OPAL developer team