# The Object Oriented Parallel Accelerator Library (OPAL)

A. Adelmann, S. Binder, Ch. Kraus, Y. Ineichen, T. Schietinger, S. Russell* and J.J. Yang**
*Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
**Los Alamos National Laboratory, Los Alamos, NM 87545*
*** China Institute of Atomic Energy, Beijing, 102413*

## Abstract

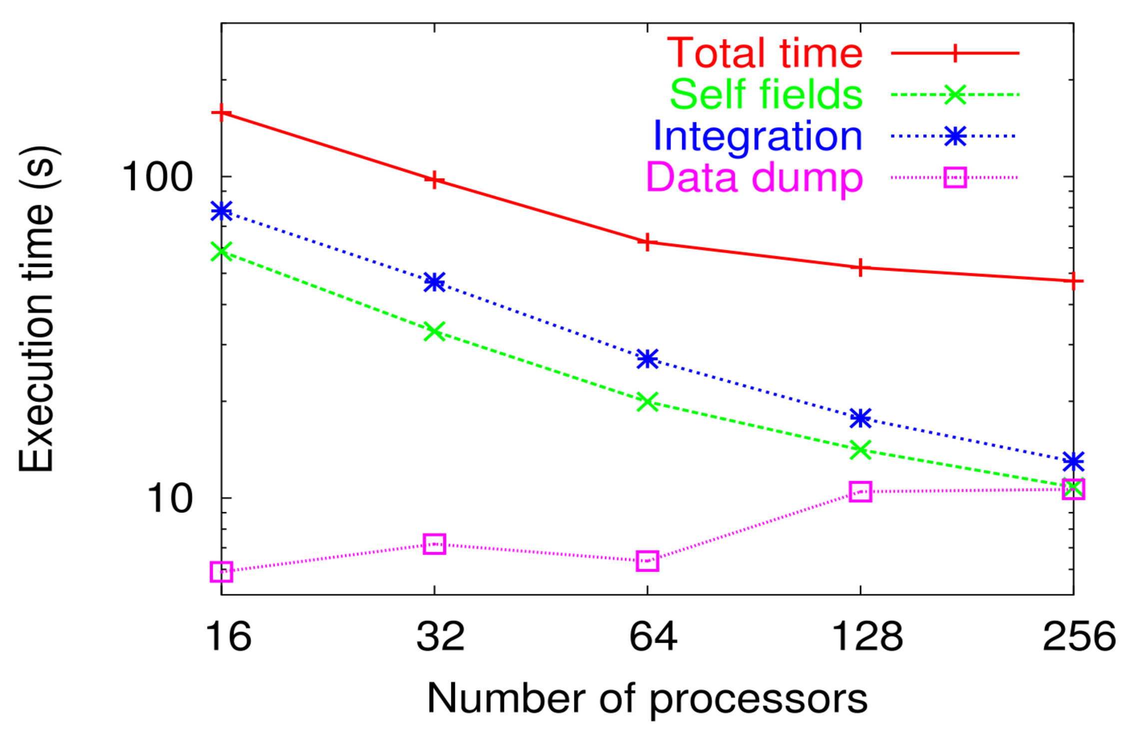
OPAL (Object Oriented Parallel Accelerator Library) is a tool for charged-particle optics calculations in accelerator structures and beam lines including 3D space charge, short range wake-fields and a 1D coherent synchrotron radiation. Built from first principles as a parallel application, OPAL admits simulations of any scale, from the laptop to the largest HPC clusters available today. Simulations, in particular HPC (High Performance Computing) simulations, form the third pillar of science, complementing theory and experiment. In this paper we present numerical and HPC capabilities such as fast direct and iterative solvers together with timings for OPAL production runs. The application of OPAL to our PSI-XFEL project will demonstrate the versatile capabilities OPAL.

## Features of OPAL

- **Time-dependent 3D parallel particle tracking code**
- **In Version 1.1.5 two flavors:**
  - **OPAL-t – linac's (SW & TW structures), beamlines, emission w. thermal emittance**
  - **OPAL-cycl – compact and separate sector Cyclotrons**
- **Built from the ground up as a parallel application runs on the laptop as well as on the largest HPC clusters (Cray XT3/4/5, IBM BG/L/P)**
- **MAD input language**
- **Collective effects**
  - **space charge (3D solver: direct FFT based & iterative SA-AMG PCG),**
  - **coherent synchrotron radiation (1D solver)**
  - **longitudinal and transverse wake fields**

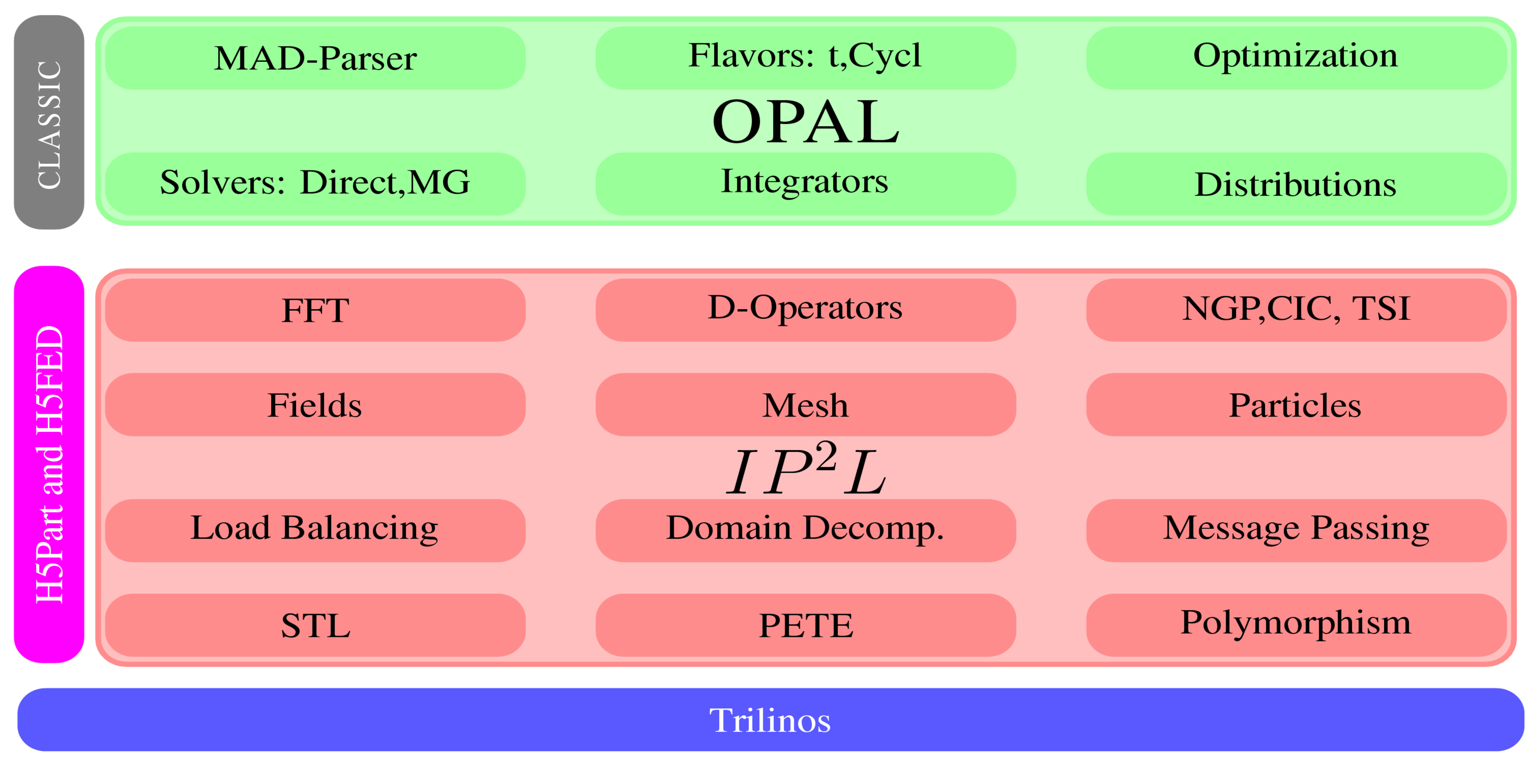
## Parallel Efficiency (Production Run)

**Space-charge solver based on integrated Green function (similar to IMPACT-T) We track $10^6$ macro-particles (Gauss distributed) on 64×64×64 mesh for 200 time steps. Dynamic load balancing and output every 10th time step.**



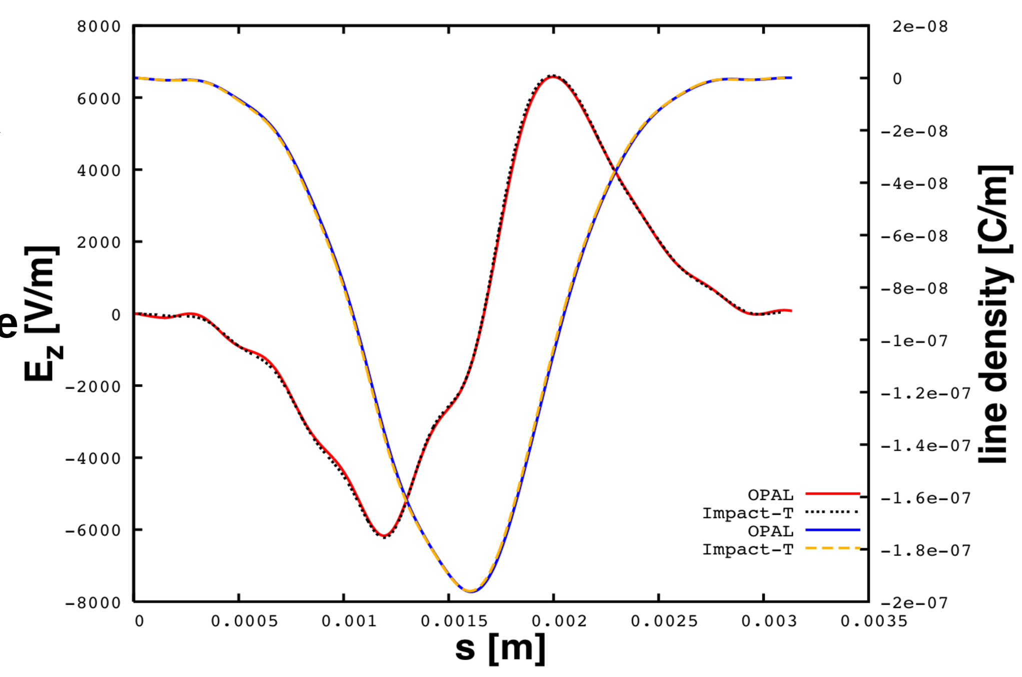

## Architecture of OPAL

**OPAL is based on several frameworks, it is object oriented, and follows the ideas of design pattern. The data parallel ansatz is provided by $IP^2L$ (Independent Parallel Particle Layer), the particle accelerator physics is encapsulated in CLASSIC (Class Library for Accelerator Simulation System and Control). The parallel I/O is based on H5Part derived from parallel HDF5. Linear solvers are provided by Trilinos.**




## Code Validation

**We have carefully benchmarked the code against IMAPACT-T and found very good agreement. Compared elements: emission including energy binning, standing and travelling wave structures, quadrupole and solenoid. Representative for the benchmarks: in a C-shaped compressor (as been foreseen in the PSI-XFEL), the z-component of the electric field of a CSR-Wake and the corresponding 1D line density is shown.**




## Example: Input File for a Phase Scan

**This is a hard calculation, scanning the phase in 2 degree steps with (energy binned) emission and full 3D space charge.**
**Such calculations are only possible with parallel computing!**

**Execute Unix commands.**

**Calculations in OPAL**

**Emission (Gauss 3D) with 10 energy bins and specially defined rise and fall time.**

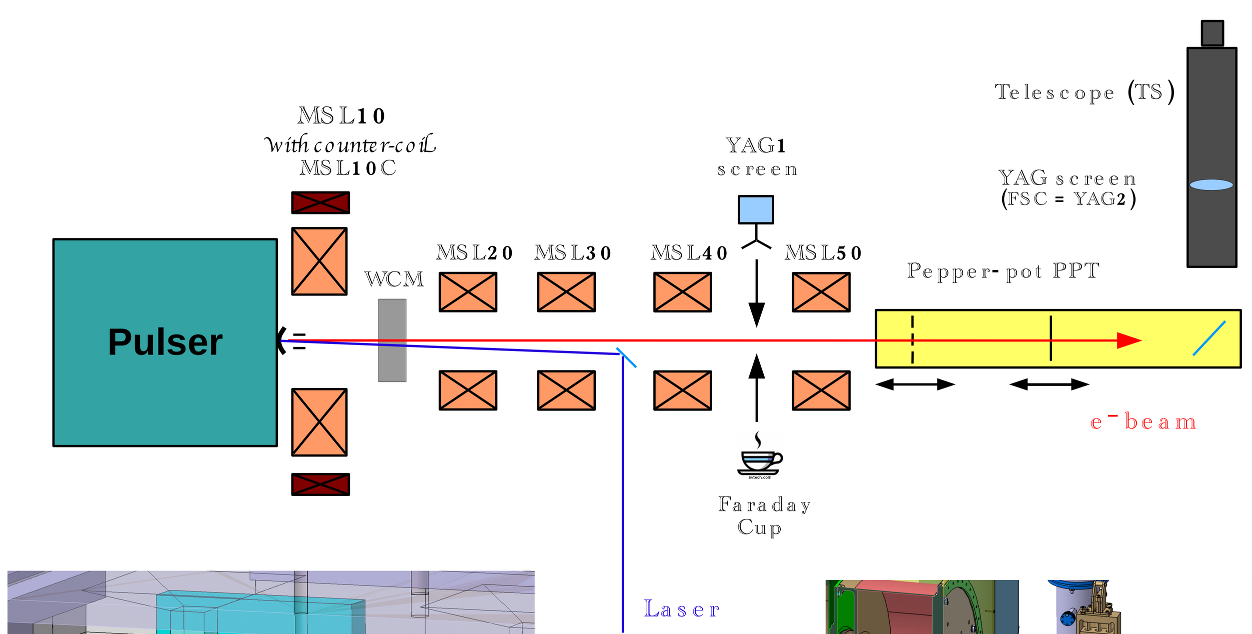
**The variable phi is changing (0,2,4 ... 360) and used to define the phase for the tracking.**

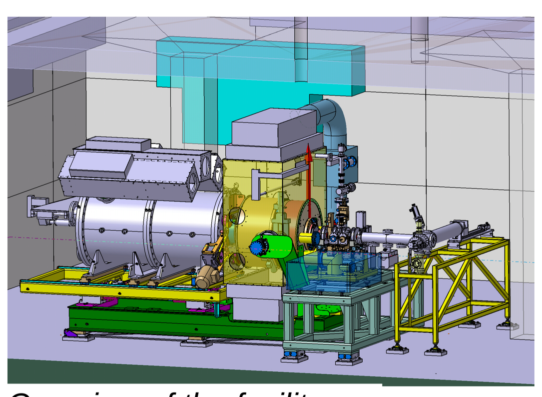
**Final energy is extracted from the output file and added to *EvsPhase.dat.***

```
Option, SCAN=TRUE;
SYSTEM,"touch EvsPhase.dat";
Title,string="OBLA 4 MeV Gun and Beam";

Edes=1.0E-9;
gamma=(Edes+EMASS)/EMASS;
beta=sqrt(1-(1/gamma^2));
gambet=gamma*beta;
P0 = gamma*beta*EMASS;
brho = (EMASS*1.0e9*gambet) / CLIGHT;
phi = 0;

v0 = beta * CLIGHT;
TRise = 0.7e-12; TFall = 0.7e-12;
TFlatTop = 9.9e-12 - TRise * sqrt(log(4)) - TFall * sqrt(log(4));
lzRise = TRise * v0; lzFall = TFall * v0;
lzFlatTop = TFlatTop * v0;

Dist1:DISTRIBUTION, DISTRIBUTION = gungaussflattop,
sigmax = 0.000540, sigmapx = 0.0, corrx = 0.0,
sigmay = 0.000540, sigmapy = 0.0, corry = 0.0,
sigmat = lzFlatTop, pt = 1.0, sigmapt = 0.0, corrt = 0.0,
risetime = lzRise, falltime = lzFall, flattoptime = lzFlatTop,
TEMISSION = 30.0e-12, NBIN = 10, DEBIN = 30;

Fs1:FIELDSOLVER, FSTYPE=FFT, MX=32, MY=32, MT=64,
                 PARFFTX=true, PARFFTY=true, PARFFTT=true,
                 BCFFTX=open, BCFFTY=open, BCFFTT=open,
                 BBOXINCR=1, GREENSF=INTEGRATED;

beam1: BEAM, PARTICLE=ELECTRON, pc=P0, NPART=10, BCURRENT=0.2997912, BFREQ=1498.956e6, CHARGE=-1;

while (phi < 360) {
 gun: RFCavity, L=0.008, VOLT=-98.954, FMAPFN="1T1.T7", ELEMEDGE=0.00,
      TYPE="STANDING", FREQ=1.0e-6;
 psl: Solenoid, L=0.12, ELEMEDGE=0.0, FMAPFN="1T2.T7", KS=0.2;
 rac: RFCavity, L=0.54, VOLT=35.5, FMAPFN="1T3.T7", ELEMEDGE=0.103,
      TYPE="STANDING",FREQ=1498.956e6,LAG=phi*RADDEG;
 sl10: Solenoid, L=1.00, ELEMEDGE=0.334, FMAPFN="1T5.T7", KS=0.133;
 sl11: Solenoid, L=1.00, ELEMEDGE=0.434, FMAPFN="1T5.T7", KS=-0.133;
 sl20: Solenoid, L=1.00, ELEMEDGE=0.834, FMAPFN="1T5.T7", KS=0.08;
 sl21: Solenoid, L=1.00, ELEMEDGE=0.934, FMAPFN="1T5.T7", KS=-0.08;

 l1:   Line = (gun,psl,rac,sl10,sl11,sl20,sl21);

 Select, Line=l1;

 track,line=l1, beam=beam1, MAXSTEPS=1600, DT=1.0e-12;
  run, method = "PARALLEL-T", beam=beam1, fieldsolver=Fs1, distribution=Dist1;
 Endtrack;

 phi = (phi+2);

 SYSTEM,"grep Emean OBLA4sim-OPAL.out > t";
 SYSTEM,"tail -1 t >> EvsPhase.dat";

}
Quit;
```

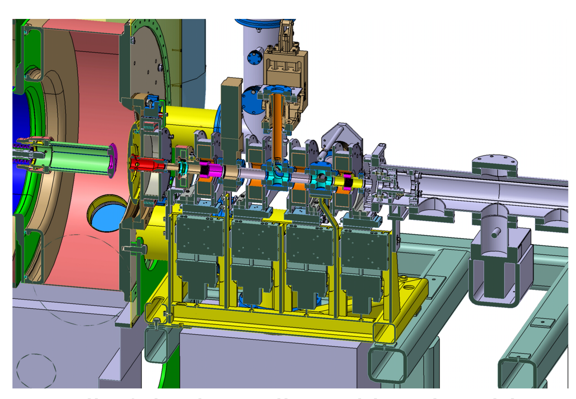
## PSI-XFEL low-emittance electron source

**OPAL is currently being used to model the low-emittance electron source test stand developed and operated in the context of the PSI-XFEL project. The electron source consists of an adjustable diode configuration subject to pulses of 250 ns (FWHM) with amplitude up to 500 kV from an air-core transformer-based high-voltage pulser.**

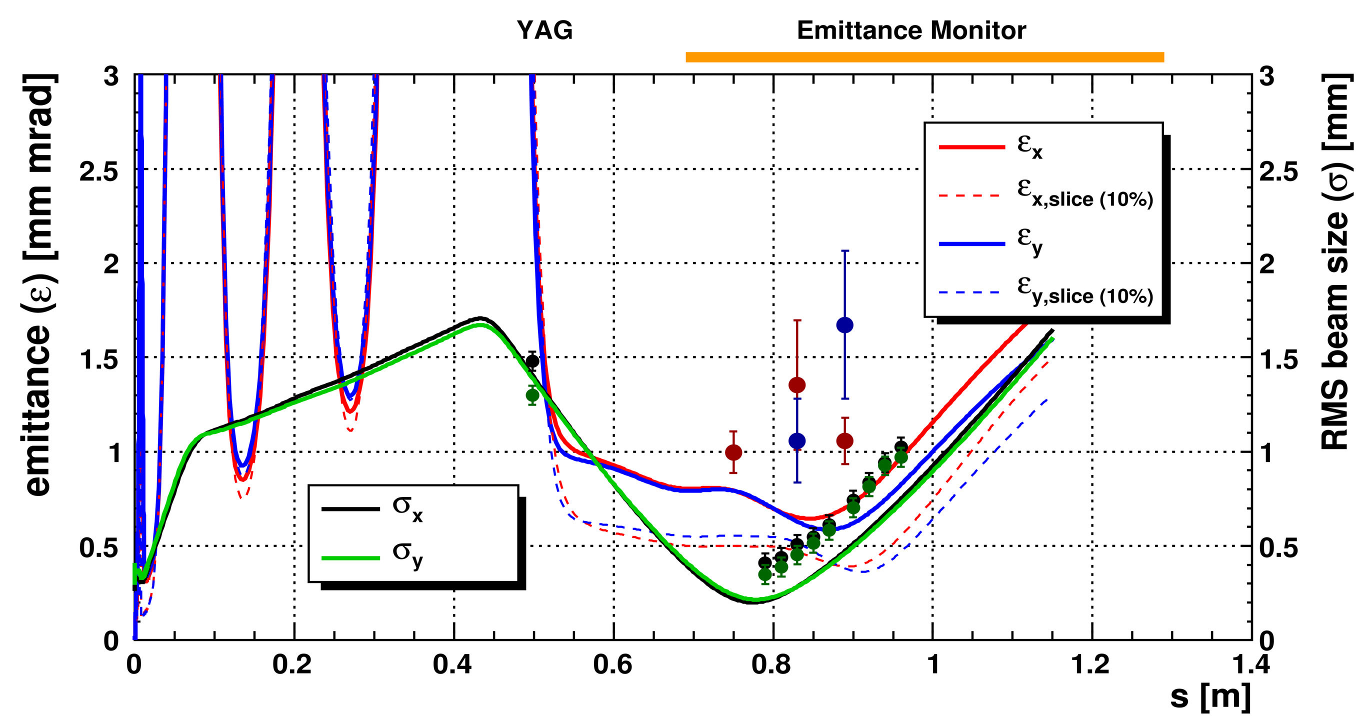


*Overview of the facility*



*Detail of the beamline with solenoids*




**Comparison of OPAL simulation results (solid and dashed lines) with measurements (points with error bars). Note that the simulated emittance does not include contributions due to thermal emittance at the cathode.**