An Update on OPAL - the Open Source Charged Particle Accelerator Simulation Framework

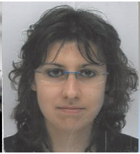
A. Adelmann for the OPAL developer team

ICAP - Key West - 23. October 2018

The OPAL Developer Team


Ch. Metzger-Kraus


S. L. Sheehy


V. Rizzoglio (*)

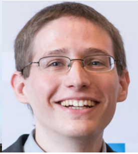

D. Winklehner

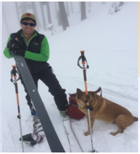

U. Locans


P. Xiaoying


J. Snuverink


A. Gsell


M. Frey (*)


S. Russel


Y. Ineichen


Ch. Rogers

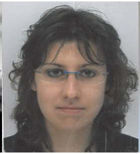

Ch. Wang


A. Adelmann

OPAL is open source ...


Ch. Metzger-Kraus


S. L. Sheehy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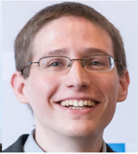
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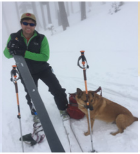

S. Russel


Y. Ineichen

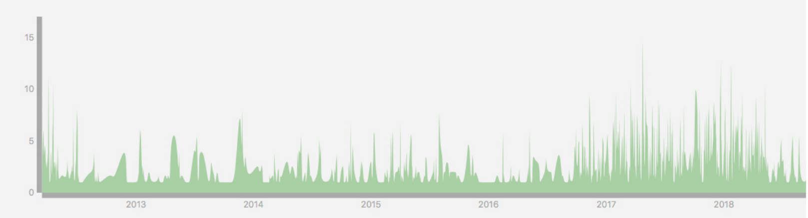

Ch. Rogers


Ch. Wang


A. Adelmann

Open Source Development

Frequency of `master` commits 2013-2018:



- hosted on gitlab.psi.ch
- anonymous read-only access with https://gitlab.psi.ch/OPAL/src.git
- write access, please contact me (andreas.adelmann@psi.ch)

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OPAL in a Nutshell I

OPAL is an open-source tool for charged-particle optics in large accelerator structures and beam lines including 3D space charge, particle matter interaction, partial GPU support and multi-objective optimisation.

- OPAL is built from the ground up as a parallel application exemplifying the fact that HPC (High Performance Computing) is the third leg of science, complementing theory and the experiment
- OPAL runs on your laptop as well as on the largest HPC clusters
- OPAL uses the MAD language with extensions
- OPAL is written in C++, uses design patterns, easy to extend
- Webpage: https://gitlab.psi.ch/OPAL/src/wikis/home
- the OPAL Discussion Forum: https://lists.web.psi.ch/mailman/listinfo/opal
- $\mathcal{O}(40)$ users

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2 OPAL flavours, OPAL-T & OPAL-CYCL released

- Common features
  - 3D space charge: in unbounded, and bounded domains
  - particle Matter Interaction (protons)
  - multi-objective optimisation
  - from e, p to Uranium (q/m is a parameter)

1. OPAL-T
   - OPAL-T with time as the independent variable, can be used to model beamlines, rf-guns, injectors
   - many more linac features like auto-phasing, wake fields, 1D CSR
2. OPAL-CYCL (+ FFAs + Synchrotrons)
   - neighbouring turns
   - time integration, 4th-order RK, LF, adaptive schemes [M. Toggweiler, AA, et al. J. Comp. Phys. 273 (2014)]
   - find matched distributions with linear space charge
   - spiral inflector modelling with space charge

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Vlasov-Poisson Equation

When neglecting collisions, and taking advantage of the electrostatic approximation, the Vlasov-Poisson equation describes the (time) evolution of the phase space $f(\mathbf{x}, \mathbf{v}; t) > 0$ when considering electromagnetic interaction with charged particles.

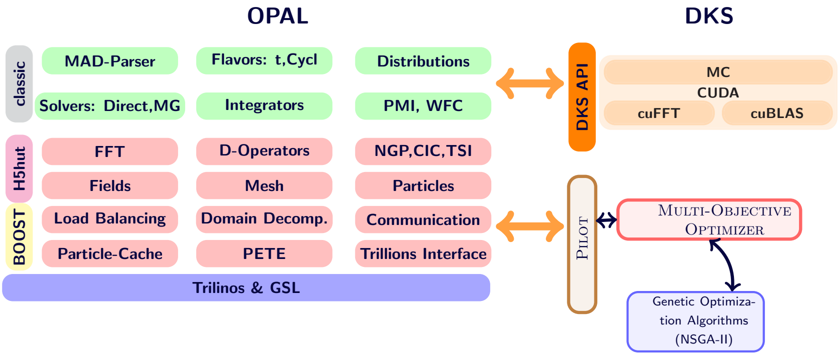
$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \frac{q}{m}(\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t)) \cdot \nabla_v f = 0. \quad (1)$$

Solving with ES-PIC

- Hockney and Eastwood, $h_x(t), h_y(t), h_z(t)$, $M = M_x \times M_y \times M_z$
- SAAMG-PCG solver with geometry [AA et al., JCP, **229** 12 (2010)]
- change M during simulation (many different field solver instances)
- adaptive in Δt
  [M. Toggweiler, AA, et al. J. Comp. Phys. **273** (2014)]
- modern computational architectures

Software Architecture

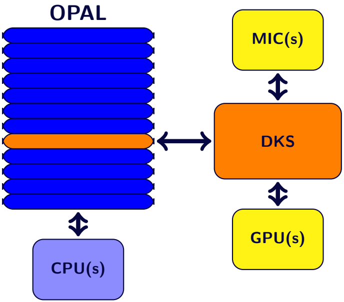
MPI based + HW accelerators + Optimiser



DKS in a Nutshell I

[AA et al., CPC **207** (2016)],[U. Locans, AA, et al., CPC **215** (2017)]

Dynamic Kernel Scheduler (DKS) is a slim software layer between host application and hardware accelerator



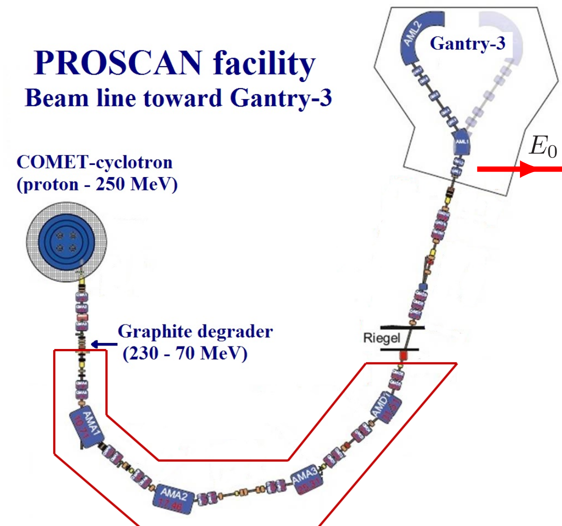
Example 1: FFT Poisson solver - results

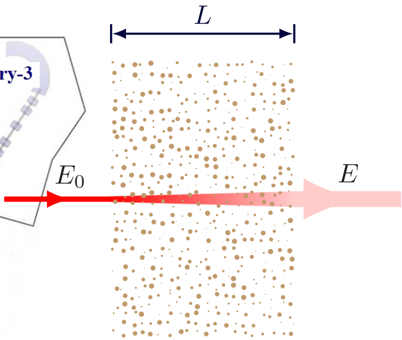
Example: simulation for the PSI Ring Cyclotron.
Host code 8 cores: 2x Intel Xeon Processor E5-2609 v2
Accelerator: Nvidia Tesla K20 or Nvidia Tesla K40

FFT size	DKS	Total time (s)	OPAL speedup	Solver t (s)	Solver speedup
64x64x32	no	324.98		22.53	
	K20	**311.17**	$\times$**1.04**	**7.42**	$\times$**3**
	K40	**293.7**	$\times$**1.10**	**7.32**	$\times$**3**
128x128x64	no	434.22		206.73	
	K20	**262.74**	$\times$**1.6**	**32.15**	$\times$**6.5**
	K40	**245.08**	$\times$**1.8**	**25.87**	$\times$**8**
256x256x128	no	2308.05		1879.84	
	K20	**625.37**	$\times$**3.6**	**202.63**	$\times$**9.3**
	K40	**542.73**	$\times$**4.2**	**160.87**	$\times$**11.7**
512x512x256	no	3760.46		3327.14	
	K40	**716.86**	$\times$**5.2**	**302.49**	$\times$**11**

Example 2: Degrader for proton therapy

[Rizzoglio et al. Phys. Rev. AB **20** (2017) , Rizzoglio et al. NIM-A **889** (2018)]





MC simulations for the degrader - results

Example: OPAL 1cm thick graphite degrader example.
Host code: 2x Intel Xeon Processor E5-2609 v2
Accelerator: Nvidia Tesla K20, K40 or Intel Xeon Phi 5110p

Particles	DKS	t_{degr} (s)	Degrader speedup	t_{integ} (s)	Integration speedup
10^5	no	20.30		3.46	
	MIC	**2.29**	×**8**	**0.89**	×**4**
	K20	**0.28**	×**72**	**0.15**	×**23**
	K40	**0.19**	×**107**	**0.14**	×**24**
10^6	no	206.77		34.93	
	MIC	**5.38**	×**38**	**4.62**	×**7.5**
	K20	**1.41**	×**146**	**1.83**	×**19**
	K40	**1.18**	×**175**	**1.21**	×**29**
10^7	no	2048.25		351.64	
	K20	**14.4**	×**142**	**17.21**	×**20**
	K40	**12.79**	×**160**	**11.43**	×**30**

Multi-Objective Optimisation with OPAL

[Y. Ineichen, AA, et al. (2012), N. Neveu, AA, et al. (2018)]

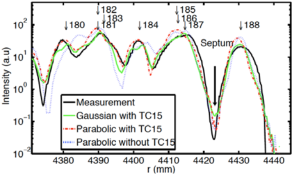
- Access to **all** OPAL statistics data as QoIs.
- Access to **all** OPAL variables as design variables
- Specify the MOOP in the OPAL input file
- Runs smoothly with more than 10000 cores

- Finds Pareto optimal solutions (NSGA-II)
- No tight coupling to parallelisation mechanism
- No tight coupling to optimisation algorithm

Selection of Past Achievements

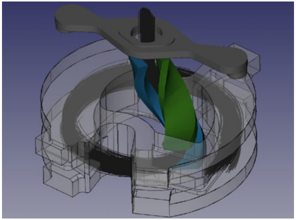
Precise high intensity cyclotron modelling

[Y. Bi, AA, et al., PR-STAB **14**(5) (2011)]



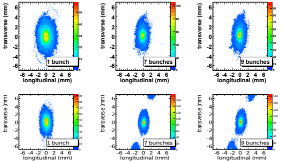
Realistic Injection Simulations of a Cyclotron Spiral Inflector

[Winklehner et al. PR-STAB **20** (2017)]



Neighbouring bunch modelling

[J. Yang, AA, et al., PR-STAB **13**(6) (2010)]

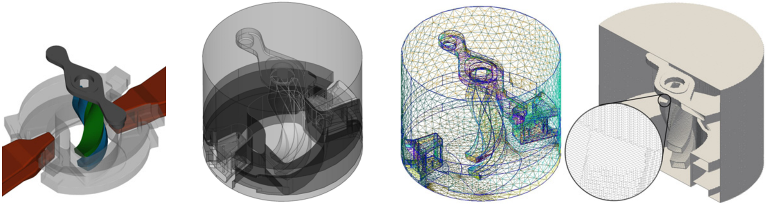


Intensity limits of the PSI Injector II cyclotron [Kolano et al. NIM-A **885** (2018)]

S2E Simulation of the DAEδALUS Cyclotron

Recently published upgrade of OPAL to perform realistic simulations of spiral inflectors [Winklehner et al. PR-STAB **20** (2017)]:

- OPAL-CYCL flavour with SAAMG-PCG solver
- Geometry loaded as *.vtk, OPAL performs initialization with voxelization for fast intersection tests at runtime
- Consider complicated spiral inflector- and grounded electrodes as boundary conditions for **field solver (mirror charges)** and **particle termination**



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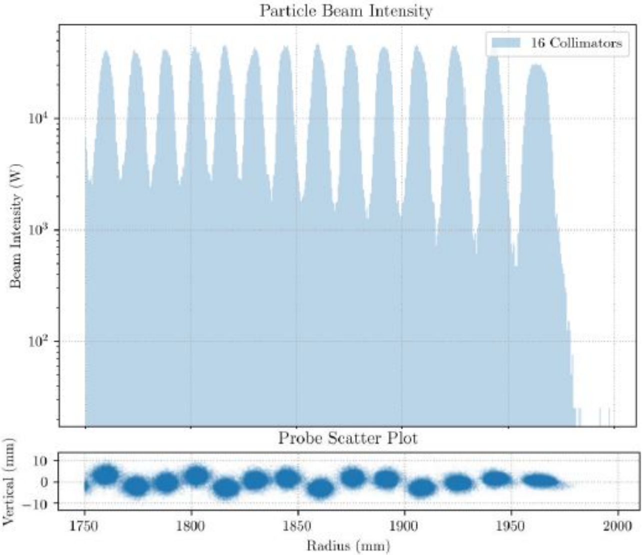

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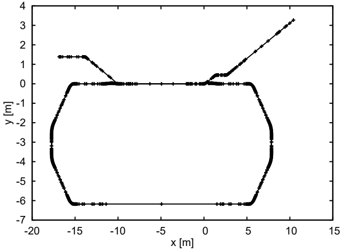
S2E ERL bERLinPro

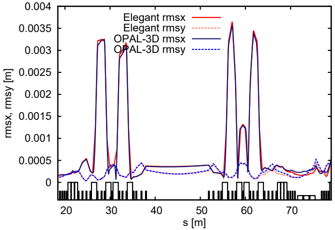
Triggered a full 3D version of OPAL-T (lead by Ch. Metzger)

Solution: place elements in 3D space.

- include all elements only once although traversed twice (n×)
- add apertures to all elements
- add origin and initial orientation of beamline (elements)

†

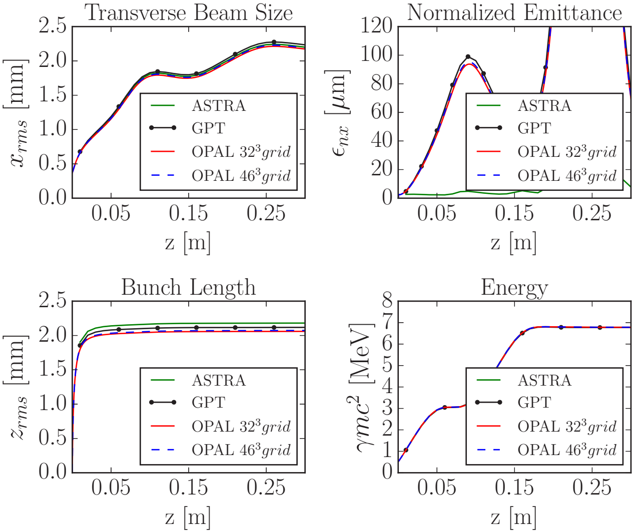




Curtesy of Ch. Metzger-Kraus (HZB), [B. Kuske, M. Abo-Bakr (2017), B. Kuske, Ch. Metzger-Kraus, Ch. Metzger-Kraus et al.]

Code Benchmarking

[N. Neveu, 2016]



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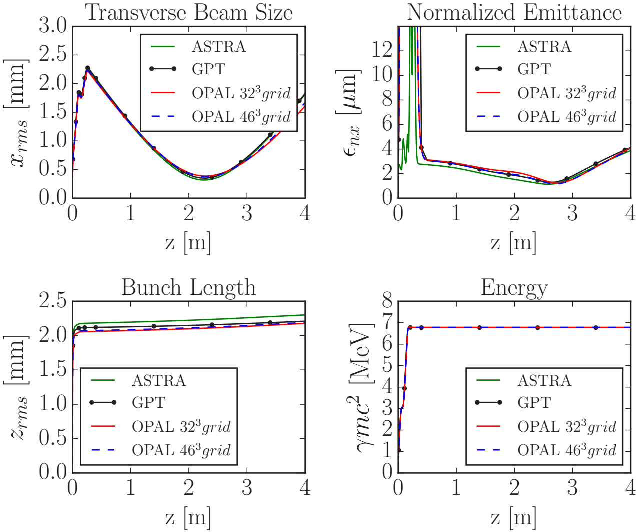
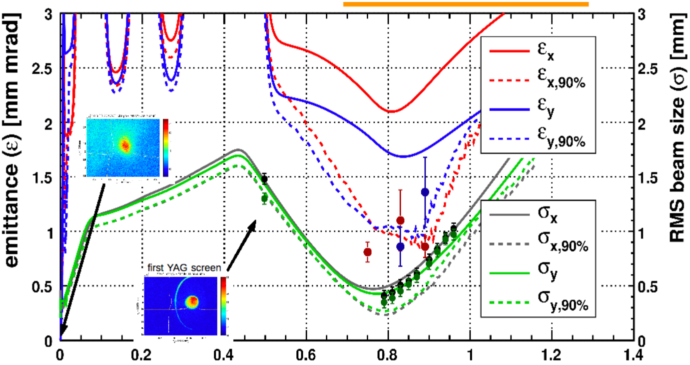


500-kV Low-Emittance Electron Source

[T. Schietinger et al., 2008]



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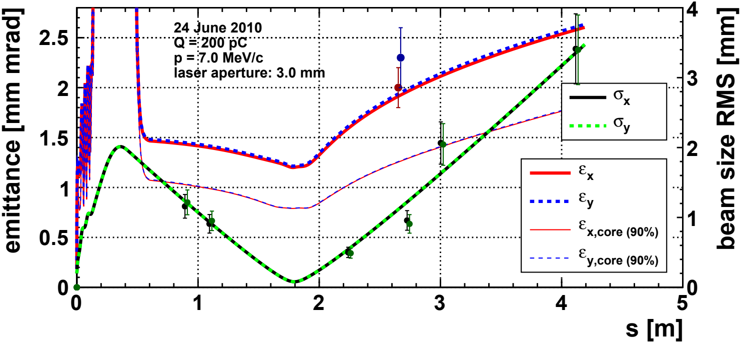
The SwissFEL Injector Test Facility Gun

[T. Schietinger et al., 2010]



Sketch of an OPAL Inputfile (only optimiser cmd's) I

AWA Photo Injector

```
dv0: DVAR, VARIABLE=P0 ,  LOWERBOUND=-10.0..
dv1: DVAR, VARIABLE=P1 ,  LOWERBOUND=-10.0 ..
dv2: DVAR, VARIABLE=G0 ,  LOWERBOUND=60.0 ..
dv3: DVAR, VARIABLE=G1,  LOWERBOUND=15.0 ..
dv4: DVAR, VARIABLE=K1,  LOWERBOUND=400.0 ..
dv5: DVAR, VARIABLE=K2,  LOWERBOUND=180.0 ..

rmsx: OBJECTIVE,EXPR=statVariableAt(rms_x ,3.1);
rmsy: OBJECTIVE,EXPR=statVariableAt(rms_y,3.1);
rmss: OBJECTIVE,EXPR=statVariableAt(rms_s,3.1);

emitx: OBJECTIVE,EXPR=statVariableAt(emit_x,3.1);
emity: OBJECTIVE,EXPR=statVariableAt(emit_y,3.1);
emits: OBJECTIVE,EXPR=statVariableAt(emit_s,3.1);
de: OBJECTIVE,EXPR=fabs(statVariableAt(dE,3.1));
```

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Sketch of an OPAL Inputfile (only optimiser cmd's) II

AWA Photo Injector

```
OPTIMIZE, INPUT="tmpl/ga-model.tmpl",
  OUTPUT="ga-model", OUTDIR="results",
  OBJECTIVES = {rmsx,rmsy,rmss,emitx,emity,emits,de},
  DVARS = {dv0,dv1,dv2,dv3,dv4,dv5,dv6},
  INITIALPOPULATION=656,
  MAXGENERATIONS=100,
  NUM_MASTERS=1,
  NUM_COWORKERS=8,
  SIMTMPDIR="tmp",
  TEMPLATEDIR="tmpl",
  FIELDMAPDIR="fieldmaps",
  NUM_IND_GEN=328,
  GENE_MUTATION_PROBABILITY=0.8,
  MUTATION_PROBABILITY=0.8,
  RECOMBINATION_PROBABILITY=0.2;
```

https://gitlab.psi.ch/OPAL/Manual-2.0/wikis/optimiser

The OPAL sampler command I

```
dv0: DVAR, VARIABLE=P0 ,  LOWERBOUND=-10.0..
dv1: DVAR, VARIABLE=P1 ,  LOWERBOUND=-10.0 ..
dv2: DVAR, VARIABLE=G0 ,  LOWERBOUND=60.0 ..
dv3: DVAR, VARIABLE=G1,  LOWERBOUND=15.0 ..
dv4: DVAR, VARIABLE=K1,  LOWERBOUND=400.0 ..
dv5: DVAR, VARIABLE=K2,  LOWERBOUND=180.0 ..

SM0: SAMPLING, VARIABLE="dv0", TYPE="UNIFORM" ..
SM1: SAMPLING, VARIABLE="dv1", TYPE="UNIFORM" ..
SM2: SAMPLING, VARIABLE="dv2", TYPE="UNIFORM" ..
SM3: SAMPLING, VARIABLE="dv3", TYPE="UNIFORM" ..
SM4: SAMPLING, VARIABLE="dv4", TYPE="UNIFORM" ..
SM5: SAMPLING, VARIABLE="dv5", TYPE="UNIFORM" ..
SM6: SAMPLING, VARIABLE="dv6", TYPE="UNIFORM" ..
```

The OPAL sampler command II

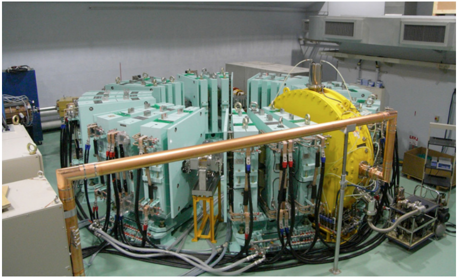
```
SAMPLE, INPUT= "rand_sample.tmpl",TEMPLATEDIR="tmpl",
    OUTPUT= "rand_sample",
    OUTDIR= "results",
    RASTER= false,
    DVARS= {dv0, dv1, dv2, dv3, dv4, dv5, dv6},
    SAMPLINGS= {SM0, SM1, SM2, SM3, SM4, SM5, SM6},
    FIELDMAPDIR= "fieldmaps",
    NUM_MASTERS= 1,
    NUM_COWORKERS= 8;
```

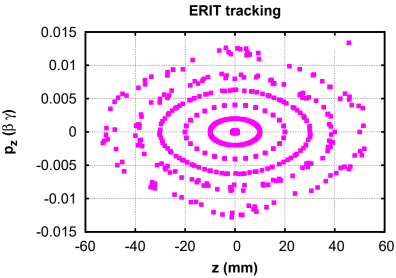
https://gitlab.psi.ch/OPAL/Manual-2.0/wikis/sampler

High Power FFA Modeling

Ch. Rogers, S. Sheey (RAL)

- ramps for rf and magnets can be specified (via. polynomial)
- analytic field scaling for FFAs
- rf fringe-fields

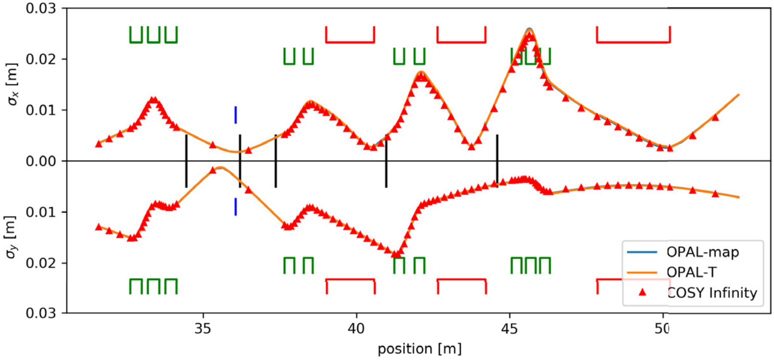




OPAL-MAP (work in progress)

PSI Gantry-2 optics (MSc. thesis P. Ganz)

- truncated power series and Lie-Methods
- maps up to arbitrary



Collisions (work in progress)

Motivation

1. model emission of ultra cold electrons
2. understand Coulomb scattering (Borsch effect) [J. Qiang, et.al]
3. do we have to worry about it in next generation machines?
4. model non Gaussian tails (high intensity hadron machines)

The

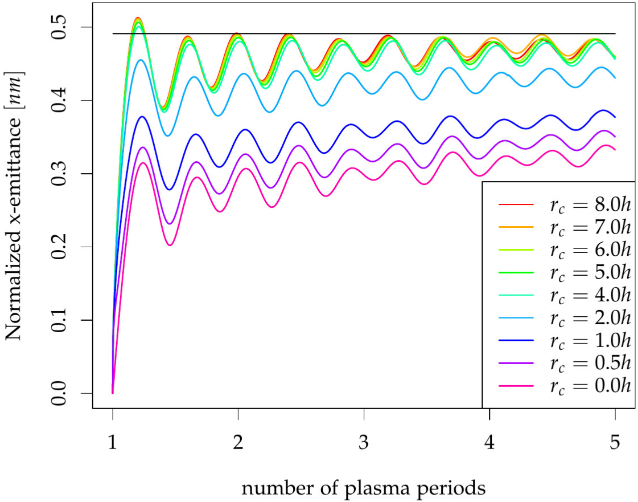
$\mathrm{P^3M}$ = **P**article-**P**article + **P**article-**M**esh

is a efficient way to accomplish this task.

- high resolution from PP part: $\mathcal{O}(K^2), K \ll N$, $1/(\boldsymbol{x} - \boldsymbol{x'} + \varepsilon)$
- good performance from PM part: $\boldsymbol{\Phi}(\boldsymbol{x}) = \int G(\boldsymbol{x}, \boldsymbol{x}')\rho(\boldsymbol{x}')d^3\boldsymbol{x}'$
- adjustable influence of Coulomb collisions by fixing K in choosing r_c

Disorder Induced Heating

Simulation Results MSc. thesis B. Ulmer



Disorder Induced Heating

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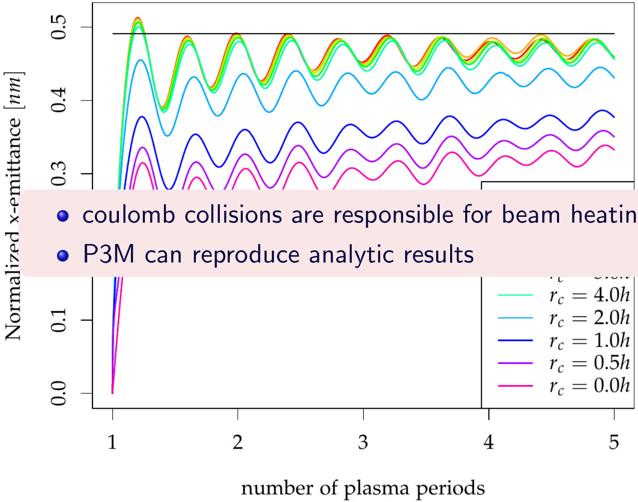

- coulomb collisions are responsible for beam heating!
- P3M can reproduce analytic results

OPAL at CPO & ICAP

- **K. Nesteruk** "Large momentum acceptance beam optics of a superconducting gantry for proton therapy"
- **N. Neveu** "Comparison of model based and heuristic optimization algorithms applied to photoinjectors using libEnsemble"
- **A. Edelen** "Surrogate models for beam dynamics in charged particle accelerators"
- **M. Frey** "Computer architecture Independent adaptive geometric multigrid Solver for AMR-PIC"
- **M. Frey** "Trimcoil optimization using multi-objective optimization techniques and HPC"
- **M. Kranjcevic** "Constrained multi-objective shape optimization of superconducting RF cavities to counteract dangerous higher order modes"

References I

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[N. Neveu, AA, et al. (2018)] , arXiv:1302.2889, 2018

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[Rizzoglio et al. NIM-A **889** (2018)] V. Rizzoglio, AA, et al. NIM-A Volume 898, 1 August 2018, Pages 1-10

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[M. Toggweiler, AA, et al. J. Comp. Phys. **273** (2014)] , J. Comp. Phys. **273** : 255-267 (2014)

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