Gun3P Top-Level Commands

- **DCGunProblem**
- **ElectrostaticProblem**
- **MagnetostaticProblem**
- **Tracker**
- **Gun3pOutputConverter**

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DCGunProblem

```
DCGunProblem:
{
  RunId: test
  SymmetryFactor: 1
  //JustGenerateTreecotree: On
  ElectricAbsoluteTolerance: 0.
  ElectricRelativeTolerance: 1.00e-12
  ElectricAbsoluteTolerance2: 0.
  ElectricRelativeTolerance2: 1.00e-12
  MagneticAbsoluteTolerance: 0.
  MagneticRelativeTolerance: 1.00e-12
  MaxIterations: 32
//  FirstIterationForMagnetostaticProblem: 1
  Save iteration data: On
}
```

DCGunProblem specifies the problem symmetry, and tolerances needed to be satisfied in order for the iterative algorithm to converge.

RunId name of the run

SymmetryFactor symmetry of the problem. 1 for full 3D, 2 for half, 4 for quarter symmetry

JustGenerateTreecotree turn this option on to generate edge trees, run on 1 core only. This does not create the output directory but only generates the Magnetostatic co Tree. Needed to use it if the problem does not converge.

ElectricAbsoluteTolerance: Absolute error always set to 0

ElectricRelativeTolerance: Relative error between consecutive iterations in the E field when magnetic solver is not activated

ElectricAbsoluteTolerance2: Absolute error always set to 0

ElectricRelativeTolerance2: Relative error between consecutive iterations in the E field when magnetic solver is activated

MagneticAbsoluteTolerance: Absolute error always set to 0

MagneticRelativeTolerance: Relative error between consecutive iterations in the H field
MaxIterations: Maximum number of iteration before the solver stops.

FirstIterationForMagnetostaticProblem: The number of iteration the magnetic solver needs to start

Save iteration data: Save data relevant to each iteration

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ElectrostaticProblem

```
ElectrostaticProblem:
{
 AnodeBoundaryId: 12
 MeshFile: dcgun.ncdf
 BasisOrder: 2
 CurvedSurfaces: on
 Charge averaging factor: 0.1
 VolumeMaterial:
 {   Id: 1
  MediumName: Vacuum
  PhysicalParameter:
  {    Name: Permittivity
   ConstantValue: 1.
  }
 }
 Write dofs to disk: on
 Debug bd dofs mapping: Off
 Debug matrix assembly: Off
 Use reduced solver: On
 Outputs:
 {
  //Matrices and vectors: On
  //Dofs for tracker: Off
    Dofs for vizualization: On
  //Dofs diff for vizualization: On
   ElectrostaticFieldToken : On
   FileName: test.data
```

```
    Nx: 40
    Ny: 50
    Nz: 60

}

Boundary:

{   Id: 1

  ConditionType: Dirichlet

  DirichletValue: 0.

}

Boundary:

{

  Id: 2

  ConditionType: Dirichlet

  DirichletValue: -500.

}

Boundary:

{

  Id: 3

  ConditionType: Neumann

  NeumannValue: 0.

}

Compute non zero initial guess: On

LinearSolver:

{

  Solver:           CG

  Preconditioner:    CHOLESKY

  PrintFrequency:    50

  QuietMode:        0

  AbsoluteTolerance: 1.00e-99

  Tolerance:        1.00e-16
```

MaxIterations: 5000

}

}

ElectrostaticProblem defines the electrostatic problem, mesh file, solver and boundary conditions

AnodeBoundaryId boundary surface ID of the Anode as defined from cubit

MeshFile mesh file generated by acdtool with format .ncdf

BasisOrder The order of the finite elements used in the simulation. Order 1-6 have been implemented. The higher the order is, the more accurate the calculation is and the more computational resources are for a fixed mesh. For most applications, using 2nd order is good enough to obtain the solution accuracy.

CurvedSurfaces on or off

The surfaces of the finite elements on the model surface are represented by curved surfaces to better approximate the geometry. If no specified, curved surfaces are used. off: The surfaces of the finite elements on the model surface are represented by flat surfaces.

Charge averaging factor: average value of the charge from one iteration to the next according to the formula

NewRays= (1 – Charge averaging factor)×PreviousRays + Charge averaging factor×NewRays

VolumeMaterial definite the electrical properties of the model

- **Id** block ID from cubit
- **MediumName**: label for the material name
- **PhysicalParameter** contains material properties for this volume
- **Name** property of the medium
    - **Permittivity:** relative permittivity of the medium
    - Permeability: relative permeability of the medium
    - Sigma: bulk conductivity of the medium units S/m
    - **ConstantValue**: value of the above property.

} }

Write dofs to disk: write electric fields

Debug bd dofs mapping: on or off. Allow debugging for advanced users. Default is off.

Debug matrix assembly: on or off. Allow debugging for advanced users. Default is off.

Use reduced solver: on or off. Reduce the number of DOFs. Default is on.

Outputs: defines output of the electrostatic solvers

- **Matrices and vectors**: Off
- **Dofs for tracker**: Off
- **Dofs for vizualization**: On
- **Dofs diff for vizualization**: Off
- **ElectrostaticFieldToken :** On or off. On allows to export the electrostatic field on a Cartesian (structured) grid to be used for Track3p.
- **FileName:** name of the file to be written
- **Nx:** number of points sampled along the x axis.
- **Ny:** number of points sampled along the y axis.
- **Nz:** number of points sampled along the z axis.

Boundary: definition of boundaries on the specified surfaces. Each boundary need a separate container.

- **Id**: surface ID as assigned in cubit
- **ConditionType**: Dirichlet or Nuemann.
- **DirichletValue**: value of the electric potential of the Dirichlet boundary
- **NuemannValue**: value of the magnetic potential of the Dirichlet boundary (usually 0)

Compute non zero initial guess: On or off. Enables non zero initial values in the 0th iteration of the electric field.

LinearSolver defines the solver for the electrostatic problem. Leave settings as is.

- **Solver**: CG for larger probmelsn

  MUMPSFLOAT for smaller problems

- **Preconditioner**: CHOLESKY
- **PrintFrequency**: 50
- **QuietMode**: 0
- **AbsoluteTolerance**: 1.00e-99
- **Tolerance**: 1.00e-16
- **MaxIterations**: 5000

}

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MagnetostaticProblem

```
MagnetostaticProblem:
{
  MeshFile: dcgun.ncdf
  BasisOrder: 2
  CurvedSurfaces: on
  Charge averaging factor: 0.1
  VolumeMaterial: {
   Id: 1
   MediumName: Vacuum
   PhysicalParameter: {
    Name: Permittivity
    ConstantValue: 1.
         }
  }
  Write dofs to disk: on
  Debug bd dofs mapping: Off
  Debug matrix assembly: Off
  Use reduced solver: On
  Outputs: {
    Dofs for vizualization: On
        }
  Boundary: {
   Id: 1
   ConditionType: Dirichlet
   DirichletValue: 0.
  }
```

```
Boundary:  {
Id: 2
 ConditionType: Dirichlet
 DirichletValue : 0
 }

Compute non zero initial guess: On
LinearSolver:
      {
            Solver:         MUMPSFLOAT
            Preconditioner:    CHOLESKY
            PrintFrequency:    50
            QuietMode:       0
            AbsoluteTolerance: 1.00e-99
            Tolerance:       1.00e-16
            MaxIterations:    5000
      }
}
```

MagnetostaticProblem defines the solver and boundary conditions for the magnetostatic solver. Follow the same syntax for the electrostatic problem.

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Tracker

```
Tracker:
{
 JobName: ./gun3p_results/OUTPUT
 Particlefile: partpath
 // For forward tracking
 t: 6.0e-6
 Generate output for vizualization: on
Print emission statistics: On
 // For backward tracking
 Backward:
 {  t: 6.0e-6
  Generate output for vizualization: on }
    Domain:
 {
  t0: 0.0
  dt: 1.0e-12
  Window_Vol: 0
  MaxImpacts: 2
 LowEnergy: 0.0
  HighEnergy: 1.0e+99
  InitialEnergy: 0.0
  dt backward: 1.0e-12
  Backward velocity pattern: 0
  Minimum backward velocity factor: 0.01
  Strategy for dt: 0
  Emission Nx:   200    //600, 300
```

```
Emission Ny:   100.   //200, 100
Emission Nz:   300.   //600, 400
Tracking Nx:   200.   //600, 300
Tracking Ny:   100.   //200, 100
Tracking Nz:   300    //600, 400
Tracking box x min: -0.11
Tracking box y min: -0.04
Tracking box z min: -0.001
Tracking box x max: 0.11
Tracking box y max: 0.04
Tracking box z max: 0.18
}
Monitor:
{
  Type: PlaneCrossingsVsT
  Name: screen
  Plane point: 0., 0., 0.15999
  Plane normal: 0., 0., 1.
  Compute densities: On
  Max x for densities: 0.110
  Max y for densities: 0.004
  X number of densities: 11
  Y number of densities: 80
}
MeshInterface:
{
  Type: pd
  Localizer:
  {
```

```
    Type: USS_Curve
  }
}
Emitter:
{
  Type: 6
  BoundaryID: 1
  t0: -1.0e-12
  t1:  1.0e-12
  N:  1.0e+0
  M:  9.10938e-31
  Q: -1.60218e-19
  d:  0.1e-3
  // 1: center
  // 2: stochastic
  Sample Type: 1
  Child Langmuir:
  {
  Whole boundary is emitter: On
 Use electric field direction for initial forward velocity: On
 Strategy: 6
 Use average J: On
 Backward velocity factor: 0.66666667
 Forward velocity factor: 1.
 Min allowed distance: 0.01e-3
 Max allowed distance: 5.00e-3
 Given delta phi: 100.0
 Max allowed emission distance wrt z axis: 1.000000
 First inter cycle factor: 1.0.
```

```
 Inter cycle averaging factor: 1.0.
 Max allowed total current: 1.35e+9
 Reference z for emission surface: 1.50e-3
 Particles per face: 5
  }
}
// HERE
Material:
{
  // 1: Reflector
  // 2: Absorber
  // 3: Secondary emitter
  // 4: Test surface
  // 5: SymmetryPlane
  BoundarySurfaceID: 1
  Type: 2
}

Material:
{
  BoundarySurfaceID: 2
  Type: 2
}
```

Tracker defines the particle tracking algorithm and solver based on the calculated electric and magnetic field for each iteration.

JobName location of the output results. Make sure it's the same name used in the job submission batch file.

Particlefile: prefix name of the particle files

T final value of the time for forward particle tracking

Generate output for visualization on or off. Generates output values for forward particle trajectories.

Print emission statistics: on or off. write emission data in the output fiel.

Backward defines backward tracking

- **t** final value of the time for forward particle tracking
- **Generate output for vizualization**: Generates output values for backward particle trajectories.

Domain tracking domain within the model

- **t0** initial time
- **dt**: time step
- Window_Vol: 0
- **MaxImpacts**: 2
- **LowEnergy**: 0.0
- **HighEnergy**: 1.0e+99
- **InitialEnergy**: 0.0
- **dt backward**: 1.0e-12
- **Backward velocity pattern**: 0
- **Minimum backward velocity factor**: 0.01
- **Strategy for dt**: 0
- **Emission Nx**: number of emission points sampled along the x axis
- **Emission Ny**: number of emission points sampled along the y axis
- **Emission Nz**: number of emission points sampled along the z axis
- **Tracking Nx**: number of tracking points sampled along the x axis
- **Tracking Ny**: number of tracking points sampled along the y axis
- **Tracking Nz**: number of tracking points sampled along the z axis
- **Tracking box x min**: minimum value of the bounding box for tracking in x
- **Tracking box y min**: minimum value of the bounding box for tracking in y
- **Tracking box z min**: minimum value of the bounding box for tracking in z
- **Tracking box x max**: minimum value of the bounding box for tracking in x
- **Tracking box y max**: minimum value of the bounding box for tracking in y
- **Tracking box z max**: minimum value of the bounding box for tracking in z

Monitor defines the monitor at which the beam parameters are calculated

- **Type** type of monitor used
  - **PlaneCrossingsVsT** a single plane monitor for particles crossing

    Name: name of monitor

    Plane point: coordinate of the plane center

Plane normal: unit vector normal to the plane

Compute densities: On or off. Compute charge density

Max x for densities: maximum value along x to compute emittances

Max y for densities: maximum value along u to compute emittances

X number of densities: number of points to emittances along x

Y number of densities: number of points to emittances along y

- **PlanesCrossing** parallel planes monitor for particles crossing each plane

  Name: name of monitor

  First plane point: coordinate of the first plane center

  Common plane normal: unit vector along the parallel planes

  Distance between first and last planes: distance between first and last planes

  Number of planes: number of planes

MeshInterface localizer interface. Keep as default.

Emitter contains all information about the emission model and boundaries for the tracker

- **Type type of emittion model**
  - 1: Thermal cathode
  - 2: MP emission mode
  - 3: Injection mode
  - 4: Test particle mode
  - 5: Window MP emission mode
  - 6: Child-Langmuir

For most gun problems we use Child-Langmuir space charge limited emission model.

- **BoundaryID** surface ID of the emitter surface(s) as assigned in cubit
- **t0**: initial time the tracker applies Lorentz force equation. Use as default.
- **t1**: final time the tracker applies Lorentz force equation. Use as default.
- **N:** number of unit particles in the macroparticle
- **M**: real mass of a unit particle
- **Q**: real charge of a unit particle
- **d**: radius of the macroparticle for space charge calculations
- **Sample Type**: 1 or 2
  - **1 emission from the center of the elements**
  - **2 emission stochastically across the elements**

- **Child Langmuir** set the emission parameters of the Child Langmuir model

- **Whole boundary is emitter**: On or off. Sets the whole boundary as emitter. Default is on.
- **Use electric field direction for initial forward velocity: On**
- **Strategy**: 6 //keep as default.
- **Use average J**: On //keep as default.
- **Backward velocity factor**: 0.66666667 //keep as default.
- **Forward velocity factor**: 1. //keep as default.
- **Min allowed distance**: 0.01e-3 //keep as default.
- **Max allowed distance**: 5.00e-3 //keep as default.
- **Given delta phi**: 100.0 //keep as default.
- **Max allowed emission distance wrt z axis**: 1.000000 //keep as default.
- **First inter cycle factor**: 1.0. //default is 0.5
- **Inter cycle averaging factor**: 1.0. //default is 0.5
- **Max allowed total current**: 1.35e+9
- **Reference z for emission surface**: this is the first point beyond the cathode at which the fields are calculated and updated on the mesh.
- **Particles per face**: 5. One can experiment with this number to obtain better convergence.

Material defines particle boundary conditions for the tracker

- **ID** surface ID as assigned in cubit
- **Type** type of surface boundary conditions for the particle
  - 1: Reflector
  - 2: Absorber
  - 3: Secondary emitter
  - 4: Test surface
  - 5: SymmetryPlane

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Gun3pOutputConverter

Gun3pOutputConverter is a post processing tool to calculate the E and H fields for a specific iteration and also output the field on structured grid (when ElectrostaticFieldToken : On)

Syntax on Perlmtter:

gun3pOutputConverter filename.gun3p e

gun3pOutputConverter filename.gun3p m

The output .mod and .data files will be stored in \gun3p_results\OUTPUT\E and \gun3p_results\OUTPUT\M