Critical analysis of numerical parameters effects
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- Feebacks from the verification and the validation cases

- Focus on the numerical parameters → higher effects on the simulation results in SPIS-Science

- Pragmatic point of view (not general and not exhaustive list)
Potentials in volume

- Boundary conditions
  - Potential on the SC (see dedicated analysis section)
  - External (or Environment) boundary conditions → physical approximation
- Space charge density (if any / second order effect in some cases)
  - Density of PIC populations (see dedicated analysis section):
    - Criterion: sufficient number of super-particles per Debye length
    - Effect: potential gradient uncertainty/ Numerical heating of the particles
    - Cause: statistical noise in a Debye length
    - Diagnostic: constant increases of the total energy of the particles
    - Solution: reduce the statistical noise on density in volume
- Boltzmann population → implicit Poisson solver
- Mesh
  - Mesh refinement
    - Criterion: resolution of the gradients of potential
    - Effect: uncertainty proportional to the mesh size / in case of space charge effect, risk of code divergence if mesh size > Debye length
    - Cause: solver fails to solve the potential gradients
    - Diagnostic: potential map not physical (high negative or positive value)
    - Solution: increase the refinement of the mesh
  - Mesh quality:
    - No criterion → not possible to estimate the error influence (Poisson solver and Complex Pusher)
    - Avoid sharp tetraedra always better
    - Diagnostic: GMSH mesh quality statistic
Potential in volume

- Solver parameters
  - Explicit solver
    - Criterion: unexplained potential variations from one step to the next step (see log console)
    - Effect: numerical inversion failure or potential oscillations in volume
    - Cause: solver precision insufficient or mesh quality insufficient
    - Diagnostic: error message or local potential oscillation
    - Solution: increase solver precision (GlobalParameters: iterGradient and tolGradient)
  - Implicit solver
    - Criterion: code divergence (very high positive or negative potential) or unexplained potential variations from one step to the next step
    - Effect: numerical inversion failure or potential oscillations in volume
    - Cause: solver precision insufficient or mesh quality insufficient
    - Diagnostic: error message or local potential oscillation
    - Solution: increase the solver precision (GlobalParameters: iterGradientNI, tolGradientNI and iterNewton and totNewton)
Potential in volume

- **Time steps**
  - Implicit electrons: no time step constraints
  - Explicit electrons:
    - Cause: PlasmaDt greater than 0.2/wpe
    - Same effect as space charge noise
    - Decrease time steps

- **Thin elements**
  - Criterion: approximation of the singularity
  - Effect: potential drop $\rightarrow$ not continuous
  - Cause: limit or out of validity of the singularity approximation
  - Diagnostic: mesh size around thin wire $\sim$ wire radius or mesh size around thin panel edges $\sim$ panel thickness
  - Solution: increase the mesh size or use mesh elements without thin approximations
Potential on SC

- Collected currents

- Emitted currents → Surface interactions

- Material properties

- Circuit solvers
  - Exact inversion (Gauss Pivot) or iterative inversion (CGS solver) of the linear system
  - Automatic switch when iterative inversion fail or user defined (implicitCircuitSolver)

- Implicitation of current collection and emission → current scaler $\frac{DI}{DV}$
  - Criterion: current prediction done correctly
  - Effect: uncertainty on potential calculation by the circuit solver / small time steps due to rapid variation of potentials / total current not zero at the stationary state
  - Cause: validity of the current scaler overestimate
  - Diagnostic: potential variations in comparison to particles energy and total current at the stationary state
  - Solution: reduce globally the validity of the current scaler (validityRenormalisation)
Collected current

- Potential on SC
- PIC populations statistics
  - Criterion: temporal noise on current collected and spatial noise on current collected map
  - Effect: uncertainty on potential calculation by the circuit solver / small time steps due to rapid variation of potential
  - Cause: insufficient number of super-particles per Super Electrical nodes surface for metal / per surface mesh element for dielectrics
  - Diagnostic: potential variation in comparison to particles energy
  - Solution: reduce the statistical noise on density in volume / improve the trajectory integration duration
- Potential map (second order)
- Volume interactions (if any)
Surface interactions

- Depends on Interactor type
  - Incoming populations
  - Material properties
  - Potential and electric field on SC
  - Mesh

- Photoemission
  - Mesh quality for self-shading

- SEEE and SEEP
  - Incoming populations
    - Criterion: current collected noise and energy/angle distribution of incoming electrons
    - Effects:
      - Current emitted affected by current collected and incoming particle energy/angle
      - Secondaries EDF affected by electron energy/angle for SEEE
    - Cause: insufficient number of super-particles per Super Electrical nodes surface for metal / per surface mesh element for dielectrics
    - Diagnostic: current collected/emitted noise
    - Solution: reduce the statistical noise on density in volume / improve the trajectory integration duration
  - Material properties
Surface interactions

- RIC
  - Incoming populations
    - Criterion: current collected noise and energy distribution of incoming electrons
    - Effects: RIC affected by energy flux calculation
    - Cause: insufficient number of super-particles per Super Electrical nodes surface for metal / per surface mesh element for dielectrics
    - Diagnostic: current collected noise
    - Solution: reduce the statistical noise on density in volume / improve the trajectory integration duration
  - Material properties
  - Potential and electric field on SC
Population in volume

- Potential map
  - Botzmann population → implicit Poisson solver
  - PIC population: trajectory integration (see dedicated section)

- Boundary conditions (particle loss or symmetry condition)

- Emitted population from SC
  - Emitted distribution accuracy (see dedicated section)
  - Emitted flux statistics:
    - Criterion: density map noise
    - Effects: local population density noise in space and time
    - Cause: insufficient number of super-particles per mesh elements
    - Diagnostic: density map or density sensor
    - Solution: increase the densification parameter of the interactor (example: electronSecondaryDensification for SEEE) / increase the statistics of current collection
Population in volume

- Population from environment:
  - Emitted distribution may depend on local potential on boundary → Potential map
  - Injection statistics
    - Criterion: density map noise
    - Effects: local population density noise in space and time
    - Cause: insufficient number of super-particles per mesh elements
    - Diagnostic: density map or density sensor
    - Solution: increase the average number of particle per cell parameter → avPartNbPerCell

- Trajectory integration (see dedicated section)
Trajectory integration

- Potential map in volume
- Mesh quality
- Solver precision
  - Exact solver → too sharp elements may induce a positioning error of the particle (Trajectory warning) due to the simple precision definition of the mesh
  - Iterative solver (in case of magnetic field, wire element or thin panel):
    - Criterion: total energy conservation during trajectory and positioning precision
    - Effects: imprecision on density in volume and current calculated
    - Cause: insufficient precision to localise the particle during the push
    - Diagnostic: warning message during the particle push / loss of particles
    - Solution: increase the precision of the pusher in position (iterativePusherAbsTolPos and iterativePusherRelTolPos) and in velocity (iterativePusherAbsTolVelo and iterativePusherRelTolVelo)