| Priority | Category | Name | Description |
|----------|--------------------|----------------------------|---|
| 1 | Documentation | DDA vs. FDTD | Mention in the manual and/or on the web site current state-of-the-art in DDA vs. FDTD |
| 2 | Usability feature | Input of fields | Implement reading of initial field of iterative solver and incident field from file. |
| 2 | Simulation feature | Calculation of Cabs | Study differerent formulations for Cabs, especially for very large refractive index. Also check, how cross sections should be calculated in the FCD framework. |
| 2 | Optimization | Optimize scattered fields | Furhter optimize calculation of the scattered field, according to the ideas of R. Scott Brock; in parallel mode distribute internal fields evenly between processors (MPI_ALLTOALLV). |
| 2 | Documentation | Adding new beam | Add a description in the appendix how to add new incident field option in the code. Do the same for adding command line options. |
| 2 | Documentation | Short name: ADDA | Change all references in the documentation and code from "Amsterdam DDA" to "ADDA". Add explanation why this is done, and send separate note to users with the next release. |
| 3 | Usability feature | Automatic testing | Implement automatic testing of releases with a wide range of command line options. This should decrease the chance of introducing new bugs into old parts/features of the code during further development. |
| 3 | Usability feature | Amplitude matrix | Implement saving of amplitude matrix (vs scattering angle) to file (together with Mueller matrix). |
| 3 | Usability feature | Formulation option | Add command line option to choose the whole formulation (like FCD, SO, LDR, etc.) |
| 3 | Usability feature | Checkpoints | Furhter development of the checkpoint system. Extend to calculations of two polarizations and orientational averaging. |
| 3 | Simulation feature | Near field | Convenient way to calculate near field in a number of points or on a grid around the particle. Possibly implement calculation of the B-field together with E-field. |
| 3 | Simulation feature | Incompl. orient. averaging | Implement calculation of scattering for the 2D grid of scattering angles (and asymmetry parameter) in combination with orientation averaging. This can be useful when orientation is not completely random. |
| 3 | Simulation feature | Continuous polarizability | Implement continuous polarizability (not discrete values, like now), change -read format accordingly. Possibly implement full tensor of polarizability. This will open way to things like Weighted Discretization. |
| 3 | Simulation feature | Polarization prescription | Implement all possible polarization prescription, at least those that are easy to do (DGF, LAK, a1-term, etc.). Think about other existing possibilities for -scat and -int options. |
| 3 | Simulation feature | Radiation forces | Completely rewrite calculation of radiation forces using FFT. Add its memory requirements to -prognose estimates, and perform other integration into the code. |
| 3 | Simulation feature | Convex Hull | Implement convex hull algorithm into shape generator to enable much wider variety of automatically generated shapes. |
| 3 | Optimization | Intel compiler | Try Intel C compiler 10.1, change Makefile if needed. |
| 3 | Optimization | Timing for MatVec product | |
| 3 | Optimization | Planning shape | Implement optimizations based on the analysis of the shape (position of real dipoles on the grid) to decrease |
| Ū | Optimization | r iaiiiiiig chapo | tests and indirect indexing in MatVec, CalcField, etc. |
| 3 | Optimization | Optimize MatVec | Optimize arithmetic operations in the MatVec function, especially the middle one (Arithm3). |
| 3 | Optimization | Optimize MPI | Several possible ways to optimize MPI part of the code: 1) use one buffer for all MPI communications; 2) possibly use MPI_ALLTOALL and 'derived datatypes' for block_transpose; 3) use 'persistent communication requests' for repeated communications. |
| 3 | Optimization | Rewrite jagged | Rewrite implementation of the -jagged option, so everything is done in the end of make_particle(). Then everything else will be automatically compatible with it. Also optimize the main cycle in make_particle. |

| Priority | Category | Name | Description |
|----------|--------------------|------------------------------|--|
| 3 | Optimization | Integration for Csca and g | Use weighting function for integration of scattered fields to obtain Csca and g. Take into account at least the diffraction peak. |
| 3 | Optimization | Determine void dipoles | Analyze dipoles with refractive index equal to unity and make them void in the beginning of the program. Also find out why it fails now, probably somewhere there is division over zero. |
| 3 | Optimization | New iterative solvers | Implement new iterative solvers, e.g. 2-term QMR and CSYM. Should improve performance for very slow convergence. |
| 3 | Optimization | Residual | Check calculation of residual inside the iterative solvers. Maybe it would be more accurate to recalculate it at the end. |
| 3 | Documentation | Citeable manual | Implement citation of the manual independently of the code, through e.g. arxiv.org. |
| 3 | Documentation | Features | Add description of features (capabilities) in the manual and on the web site. |
| 3 | Documentation | Euler angles | Add specific definition (with figures) of the used notation for Euler angles in the manual. |
| 3 | Documentation | Surrounding medium | Explain the transformation of the radiation forces due to the surrounding medium in the manual. |
| 4 | Usability feature | Single polarization | Implement simulation for single given incident polarization (complex amplitude). It will cut down simulation time twice for certain applications. |
| 4 | Usability feature | Binary shapes | Implement binary format for shape files, which can save space tremendously for homogeneous particles. |
| 4 | Usability feature | Shape information | Save more information about the shape, when using -save_geom. |
| 4 | Simulation feature | Revise 'box' shape | Possibly revise the definition of box in 'box' and 'spherebox' shapes. |
| 4 | Simulation feature | New shapes | Implement general shapes like 'coated ellipsoid', 'boxsphere', 'spherebox' with a lot of input parameters. |
| 4 | Simulation feature | Spectrum | Implement convenient simulation of spectrum, either inside of ADDA, or with a separate script. Possibly optimize calculation by simultaneous solving for many wavelength values in one iterative sequence (should be especially relevant in case of Rayleigh particles). |
| 4 | Simulation feature | Rayleigh limit | Implement special Rayleigh mode, which enables some simplifications (like using CG iterative solver and calculating only total polarizability tensor). Use additional symmetries of the particle (rotation around y and x axes by 90 degrees). |
| 4 | Simulation feature | SO formulation | Further develop SO formulation, bring it out of the development phase. |
| 4 | Optimization | Shared-memory | Optimize ADDA for shared memory hardware (e.g. multi-core processors), using standard MPI functions. |
| 4 | Optimization | FFTW upgrade | Implement certain parts of the code using MPI functions in FFTW 3.2, either the whole 3D FFT transforms, or local and MPI transpose operations. |
| 4 | Optimization | Sphere quadrature | Implement orientation averaging using quadrature over sphere surface, according to ideas of Antti Penttila. |
| 4 | Optimization | Memory in prognose | Ensure then when -prognose option is used, minimum memory is allocated in make_particle(). |
| 4 | Optimization | Accumulate alpha | Optimize accumulate function (parallel communication) when averaging over alpha angle. Do all communication at once and do not use unnecessary memory (Eplane <=> ampl_alpha). |
| 4 | Optimization | Overflow of clock | Try to avoid overflow of 'clock' function when run in a sequential mode. |
| 4 | Optimization | One polarization per orient. | Reformulate orientational averaging so that only one incident polarization per orientation is simulated. |
| 5 | Usability feature | Incident angles | Implement specifying incident propagation direction by two angles istead of Cartesian coordinates of the vector of incidence. |
| 5 | Usability feature | Accurate memory counting | Make memory accounting more accurate, include non-major contributions and take into account dynamic allocation/deallocation. |

| Priority | Category | Name | Description |
|----------|--------------------|----------------------------|---|
| 5 | Simulation feature | Multi-grid | Implement multi-grid DDA, according to the ideas of Vitezslav Karasek, for simulation of clusters of particles, which are at considerable distances from each other. |
| 5 | Simulation feature | Van der Mee & Hovenier | Implement Van der Mee & Hoveniers test on the Mueller matrix. Probably makes real sense only for the results of orientational averaging. |
| 5 | Optimization | Reduced D matrix | Optimize storage of D matrix to use less memory (at least in sequential mode). |
| 5 | Optimization | Optimize scattered fields | Further optimize scattered field calculation for large grid of angles, trying to use FFT-based ideas to transforming 3D array of polarizations to a sphere surface in spectral space. |
| 5 | Optimization | Fields from smaller dpl | Use internal fields from smaller dpl as an input for the iterative solver of a simulation with larger dpl. The general methodology is described somewhere in Numerical Recipes. |
| 5 | Optimization | Optimize two polarizations | Possibly use the internal field obtained for one incident polarization to cut down the number of iterations for the second. |
| 5 | Optimization | Reuse orientation | Reuse calculated internal fields from one orientation for the similar ones to speed up orientation averaging. |
| 5 | Optimization | Ci,Si | Optimize calculation of sine and cosine integrals, e.g. implement code from gsl. |
| 5 | Optimization | Optimize Mueller matrix | Optimize calculation of the Mueller matrix from the amplitude matrix. |
| 5 | Optimization | ReducedFFT and CS | Study the combination of reduced FFT and Complex Symmetric iterative solvers. Possibly implement automatic detection of some non-viable combinations. |
| 5 | Optimization | Accelerate D matrix | Optimize calculation of D matrix, especially relevant when FCD or SO is used. |
| 5 | Optimization | WKB initial field | Use internal field from WKB approximation as an input for the iterative solver. |
| 5 | Optimization | MatVec and 'her' option | Check that 'her' works fine in combination with not_reduced FFT. Maybe in this case matrix need to be duplicated in parallel mode. |
| 5 | Optimization | Linear algebra | Take a look on LAPACK, may be it can accelerate linear operations on large arrays. |