ADVANCES IN PARALLEL ELECTROMAGNETIC CODES FOR ACCELERATOR SCIENCE AND DEVELOPMENT

Kwok Ko, Arno Candel, Lixin Ge, Andreas Kabel, Rich Lee, Zenghai Li, Cho Ng, Vineet Rawat, Greg Schussman and Liling Xiao, SLAC, Menlo Park, CA 94025, USA

Abstract

Over a decade of concerted effort in code development for accelerator applications has resulted in a new set of electromagnetic codes which are based on higher-order finite elements for superior geometry fidelity and better solution accuracy. SLAC's **ACE3P** code suite is designed to harness the power of massively parallel computers to tackle large complex problems with the increased memory and solve them at greater speed. The US DOE supports the computational science R&D under the SciDAC project to improve the scalability of **ACE3P,** and provides the high performance computing resources needed for the applications. This paper summarizes the advances in the **ACE3P** set of codes, explains the capabilities of the modules, and presents results from selected applications covering a range of problems in accelerator science and development important to the Office of Science.

3D ELECTROMAGNETIC SOFTWARE

The advent of 3D electromagnetic (EM) codes for accelerator applications can be credited to Thomas Weiland who developed the "Finite Integration Technique" (FIT) and implemented in the **MAFIA** code suite based on a finite difference (FD) structured grid, which is now the commercial package **Microwave studio** by CST GmbH. Also FD based is **GdfidL** which is a parallel code for time varying and resonant fields. Other common commercial codes for high frequency simulation include **HFSS** from Ansoft and **ANSYS** from ANSYS, Inc. using the finite element (FE) method on an unstructured mesh. All these codes are available on parallel platforms. This paper presents the advances in the **ACE3P (A**dvanced **C**omputational **E**lectromagnetic **3D** **P**arallel) software which is a higher-order FE code suite developed at SLAC, capable of using massively parallel computations (>10k CPUs) to model large accelerator structures with higher accuracy.

PARALLEL CODE DEVELOPMENT AT SLAC

The code development effort of **ACE3P** started with a PhD thesis research [1] more than a decade ago to explore the parallel FE approach for electromagnetics in accelerator modeling. This led to the support from DOE's High Performance Computing (HPC) programs under the Accelerator Grand Challenge (1998–2001), followed by the Accelerator Science and Technology (AST) project under the Scientific Discovery through Advanced Computation SciDAC-1 program (2001-2007), and continuing as the Community Petascale Project for Accelerator Science and Technology under SciDAC-2 (2007-2012) [2,3,4].

The motivation to develop highly accurate codes for modeling complex accelerator structures originated from the machine R&D for the ILC for which SLAC is a principal proponent. To meet the requirements for beam stability, the dimensions of the ILC accelerator cavity shown in Fig. 1 need to be modeled to 0.01 % accuracy in frequency so that tuning in the fabrication process can be avoided to reduce cost. There are several challenges to this task: (1) complexity of the HOM coupler with fine feature versus the cavity size, (2) problem size of multi-cavity structure and cryomodule, (3) required accuracy of 10s of kHz mode in a GHz range, and (4) speed for fast turnaround time to impact design.

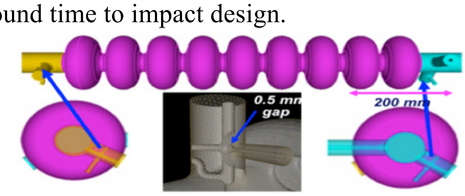

Figure 1: The ILC SRF cavity.

PARALLEL HIGHER-ORDER FE METHOD

In view of the ILC cavity modeling requirements, the **ACE3P** codes are developed based on the parallel higher-order FE method. A key advantage of the conformal (tetrahedral) mesh over the FD structured mesh is geometry fidelity as shown in Fig. 2a for the example of a coupler cavity. Further accuracy can be obtained through the use of quadratic surface and higher-order elements (p = 1-6) resulting in reduced computational cost as seen in Fig. 2b. An equaling important advantage is the power of parallel processing which both increases memory and speed, allowing large problems to be solved in far less time through scalability. Finally but not least, the success of large-scale simulations through high performance computing (HPC) relies heavily on the computational science research funded by SciDAC to improve code scalability and produce the desired results.

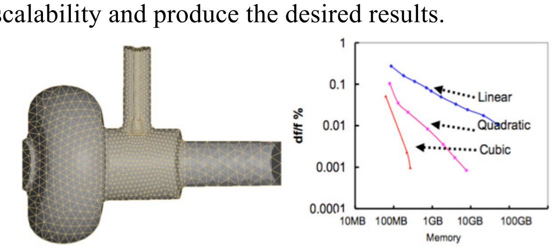

Figure 2: (a) Tetrahedral mesh of a coupler cavity; (b) Frequency convergence of a cavity mode in terms of computer memory usage using p = 1, 2 and 3 basis functions in elements.

ACE3P CODE SUITE AND CAPABILITIES

All electromagnetic modeling requires three standard steps which are building models and meshing, applying solvers and post processing. We use **CUBIT** for building CAD models and generating finite-element meshes http://cubit.sandia.gov, **ACE3P** to obtain the solutions https://slacportal.slac.stanford.edu/sites/ard_public/bpd/acd/Pages/Default.aspx, and **ParaView** for visualization http://www.paraview.org/.

ACE3P consists of the following modules: **Omega3P** for calculating cavity modes and damping, and **S3P** for transmission in open structures in frequency domain; **T3P** for calculating wakefields and transients in time domain; **Track3P** for multipacting and dark current studies using particle tracking; and **Pic3P** for RF gun design with particle-in-cell (PIC) method.

Many capabilities of **ACE3P** have been developed to cover the needs of accelerator design. **Omega3P** [5] can be used to optimize RF parameters, reduce peak surface fields, calculate HOM damping, find trapped modes and their heating effects, design dielectric & ferrite dampers, and others. **S3P** calculates S parameters. **T3P** [6] evaluates broadband impedance, trapped modes and signal sensitivity with a driving beam, computes wakefields of short bunches using a moving window, and simulates beam transits in large 3D complex structures. **Track3P** [7] studies multipacting in cavities & couplers by identifying MP barriers, and computes dark currents in accelerating structures. Finally **Pic3P** [6] calculates beam emittance in RF guns.

COMPUTATIONAL SCIENCE AND HPC

For **ACE3P** to fully apply its capabilities, it is essential that the codes can efficiently and effectively use the resources made available through SciDAC to support the R&D in computational science, and by way of computer allocations at the two DOE flagship computer centers at NERSC (LBNL) and NCCS (ORNL).

The computational science R&D for **ACE3P** includes algorithms for improving the speed and scalability of the eigensolver in Omega3P (Fig. 3), mesh correction schemes to reduce modeling errors (Fig. 4), new partitioning methods for better load balancing, and automatic adaptive mesh refinement to optimize computing resources (Fig. 5).

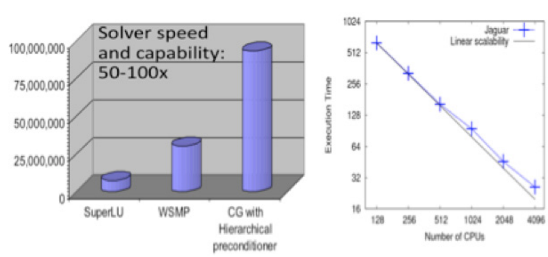

Figure 3: (a) Speed improvement for various eigensolvers; (b) Scalability of Omega3P on Jaguar (NCCS).

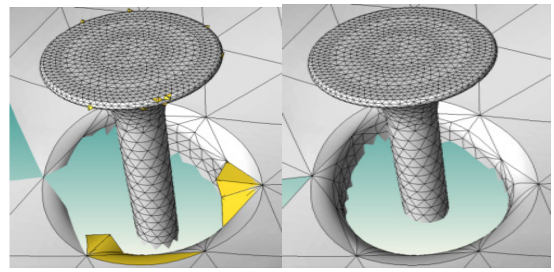

Figure 4: (a) Mesh with invalid tetrahedrons (yellow) generated from **CUBIT**; (b) Mesh after applying mesh correction tools.

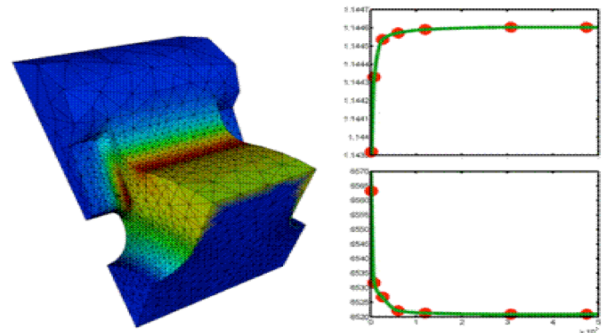

Figure 5: (Left) Field distribution of a cavity mode in the final mesh after adaptive refinement. (Right) Convergence of frequency (top) and Q (bottom) at different levels of mesh refinement.

The HPC facilities at NERSC and NCCS accessible to accelerator modeling are Franklin (Fig. 6a) which is a Cray XT4 with 38642 compute cores, 77 TBytes memory and rated at 355 Tflops, and Jaguar (Fig. 6b) which is a Cray XT5 with 224,256 compute cores, 300 TBytes memory, 600 TBytes disk space and rated at 2331 TFlops, respectively.

The computer time allocation for **ACE3P** simulations from NERSC includes 1M CPU hours, (renewable) for the *Advanced Modeling for Particle Accelerators* project, 1.6M CPU hours (renewable and shared) for the *SciDAC ComPASS* project, and 300K CPU hours for the *Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators* project (renewable and shared). From the NCCS, the allocation is 12M CPU hours in FY10 for the *Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling* project.

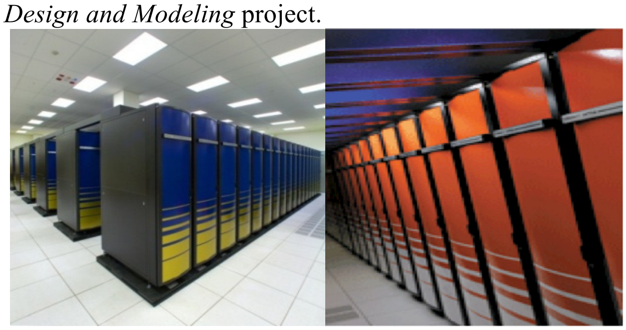

Figure 6: (a) Franklin at NERSC; (b) Jaguar at NCCS.

ACE3P COMPARISONS WITH MEASUREMENTS

(1) The cell design effort in 2001 for the JLC/NLC X-Band structures required that the 3D cavity dimensions be accurate and better than machining tolerance. The structure cells were high-precision machined and **Omega3P** was used to determine the cell dimensions. Microwave QC verified cavity frequency accuracy to 0.01% relative error (1MHz out of 11 GHz) as required for beam stability.

Omega3P also provided the dimensions for the LCLS RF gun cavity that met design requirements. This cavity employs a 3D racetrack dual-feed coupler design to minimize the dipole and quadrupole fields and reduce pulse heating by rounding of the z-coupling iris (Fig. 7). There is remarkable agreement between the design and measured RF parameters: π mode frequency in GHz (2.855987 vs 2.855999), Qo (13960 vs 14062), β (2.1 vs 2.03), mode separation in MHz (15 vs 15.17) and field balance (1 vs 1), validating the accuracy of the code [8].

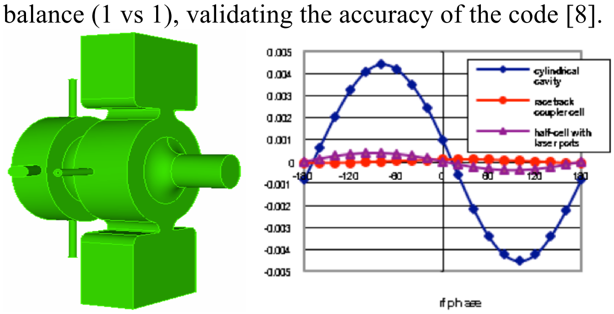

Figure 7: (Left) LCLS RF gun; (Right) Quadrupole moment in the gun cavity.

(2) The Ichiro cavity experienced low achievable field gradient and long RF processing time. Computations using **Track3P** predicted a hard barrier at 29.4 MV/m field gradient with multipacting in the beampipe step which was confirmed by measurements.

During the operation of the SNS superconducting linac, abnormal signals were observed at the HOM coupler of the β=0.81 cavity. Multipacting was suspected to be the cause of the anomaly so **Track3P** was used to analyze the problem. A scan for the multipacting activity shows two MP bands in the gradient range up to 20 MV/m which are in good agreement with experimental observations (Fig. 8).

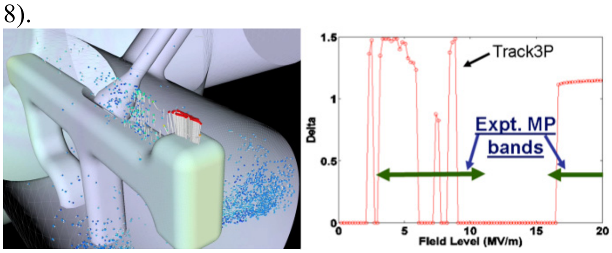

Figure 8. (Left) Multipacting activities in the SNS HOM coupler; (Right) Comparison of MP bands with measurements.

LARGE-SCALE SIMULATIONS WITH ACE3P

(1) Simulating the ILC Cryomodule

Omega3P was used to calculate the trapped modes in the ILC cryomodule which consists of eight TTF cavities. Of particular interests are the dipole modes above the beampipe cutoff frequency as they extend over multiple cavities. Sixteen dipole modes with high shunt impedance were evaluated and the damping factors were found to agree reasonably well with the measured data at DESY. This first-ever calculation on the cryomodule scale is important for the understanding of the wakefields and higher-order-mode (HOM) effects in the ILC (Fig. 9).

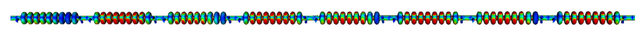

Figure 9: A mode in the third dipole band in the ILC cryomodule.

In the time domain, the beam transit in the ILC cryomodule was simulated using **T3P** with a bunch length longer than the nominal. A snapshot of the beam excited fields in the cavities and the HOM couplers is shown in Fig. 10. The simulation was carried out on the Jaguar at NCCS using 8192 cores for a problem requiring 500M degrees of freedom.

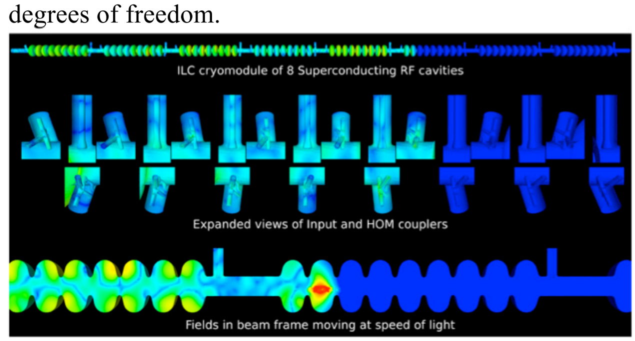

Figure 10: A snapshot of the transit of a Gaussian bunch through the ILC cryomodule.

(2) Wakefield coupling in CLIC two-beam module

CLIC's two-beam accelerator concept envisions RF power transfer to the accelerating structures from a separate high-current decelerator beamline consisting of power extraction and transfer structures (PETS). It is essential that this novel scheme be verified through simulation to understand the fundamental and higher-order mode properties in and between the two beam lines. **T3P** is used to simulate the transverse wakefield coupling between them and Fig. 11 show the first-ever results for such calculations using a simplified coupled model of the PETS and two TD24 accelerating structures [9]. The simulation is initiated with a single drive beam at an offset in the PETS and excites transverse wakefields that couple to the TD24. The evolution of the transverse electric field magnitude along the axis of the TD24 as a function of time is shown in Fig. 11. The computation required 10 hours on 12,000 cores on Jaguar at NCCS.

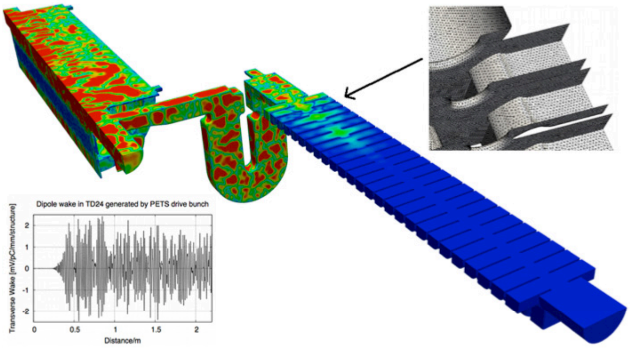

Figure 11: Snapshot of wakefield coupling simulation of the CLIC Two-Beam Accelerator, performed with T3P. A single drive beam in the PETS (left structure) is used to exciting dipole wakefields that couple to the TD24 accelerating structure (right structure), in combination with electric boundary conditions in the horizontal symmetry plane. A detailed view of the unstructured conformal (curved) mesh model is shown on the top right. The resulting wake potential is shown in the bottom left.

(3) Short-range wakefields in PEP-X

For the storage ring As a next generation synchrotron light source, PEP-X requires the calculation of wakefields at ultra-short bunch length in long 3D beamline components which is a computational challenge. Such a case is the undulator structure for PEP-X which consists of a long smooth taper that connects vacuum chambers with different cross sections on either side (Fig. 12). The structure length is 0.3 m, which is much longer than the RMS bunch length of 0.0005 m. Because of the disparate length scales the moving technique in **T3P** is used to significantly reduce the computational resources required for the simulation [10]. Fig. 13 shows the wakefield for 0.5 μm bunch and the comparison of a 3 mm bunch with that reconstructed from 0.5 μm. The excellent agreement confirms the calculation with the short bunch. This computation took 15 CPU hours using 6000 cores on Jaguar to obtain the results with the desired accuracy.

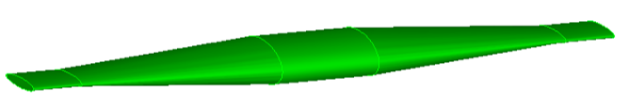

Figure 12. Model of the PEP-X undulator taper structure.

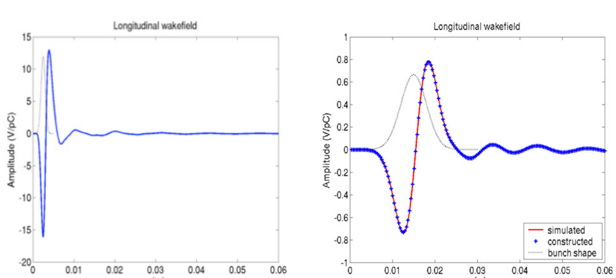

Figure 13. (Left) Short-range wakefield for the PEP-X undulator with a RMS bunch length 0.5 μm. (Right) Comparison of wakefield for 3 mm bunch with that reconstructed from 0.5 μm.

(4) Emittance calculation of X-band RF gun

The SLAC/LLNL X-band photocathode RF gun is simulated with **Pic3P** by solving the full set of Maxwell-Lorentz equations. All pertinent physics such as space-charge, image charge, retardation and wakefield effects are included self-consistently [6]. A full-3D simulation is carried out to calculate the emittance growth due to a transverse laser spot offset A snapshot of the space-charge fields and emittance results for various bunch offsets (in the direction of the coupler) are shown in Figure 14.

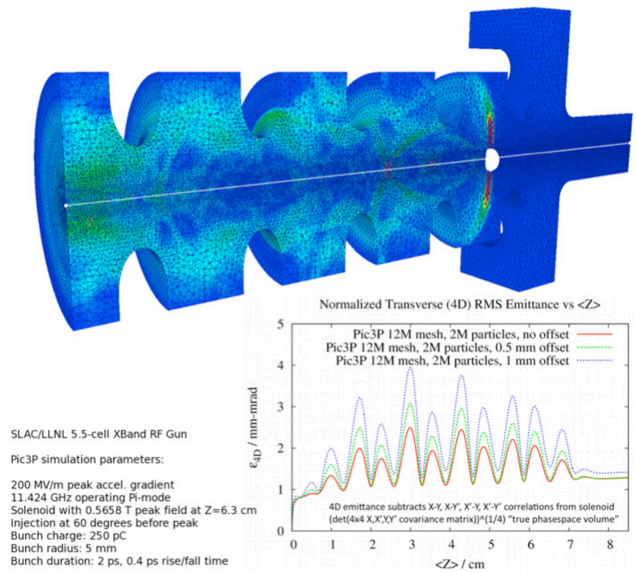

Figure 14: Emittance computations for the SLAC/LLNL X-band RF gun with **Pic3P** [11]. Magnitude of the electric space-charge field is shown for an off-center particle bunch, with resulting emittance growth (bottom).

SOLVING THE CEBAF BBU

In the CEBAF 12-GeV upgrade, beam breakup (BBU) was observed at beam currents well below the design threshold. Using measured RF parameters such as frequency, Qext, and mode field profile as inputs, the solutions to the inverse problem identified the main cause of the problem by recovering the true shape of the cavity. Due to fabrication errors, the cavity was 8 mm short as predicted and confirmed later from measurements (Fig. 15). Because of this deviation from the designed shape, three cavity modes are shifted away from the coupler and not damped effectively resulting in the abnormally high Qs (Fig. 16). The effort to resolve the CEBAF puzzle showed that experimental diagnosis, advanced computing and applied mathematics working together solved a real world problem as intended by SciDAC [12,13].

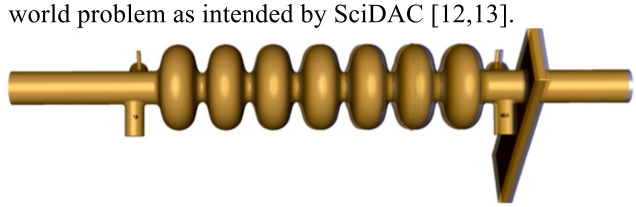

Figure 15: The CEBAF SRF original (silver) and deformed (gold) cavities.

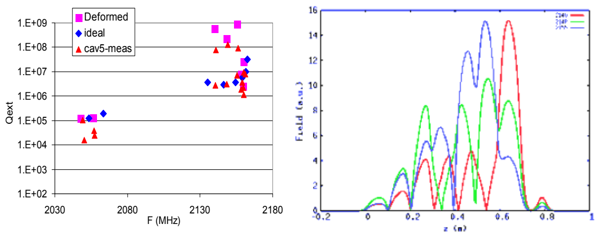

Figure 16: (Left) Qs of dipole modes for the calculated ideal cavity, deformed cavity and measurement; (Right) Field distributions of the high Q dipole modes shifted away from the HOM couplers and reduced damping.

Methods for solving the inverse problem based on nonlinear iterations with Newton type algorithms have been further developed to solve optimization problems. The method has been applied to optimize the performance of the choke mode cavity under the standard cavity design constraints of frequency and mode balance with the goal function to reduce the effects of higher-order dipoles modes to a minimum [14]. Fig. 17 shows a much lower field in the optimized cavity versus the original design that corresponds to a lower Q and higher damping.

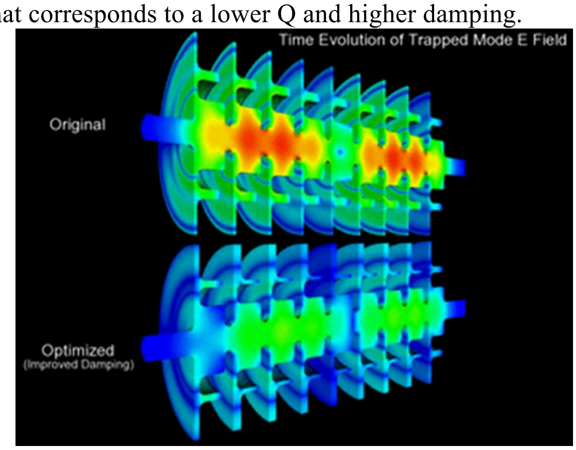

Figure 17: The field distribution choke-mode cavity: (Top) Original design; (Bottom) Optimized design.

SUMMARY

(1) Parallel finite-element (FE) electromagnetics (EM) method demonstrates its strengths in high-fidelity, high-accuracy modeling for accelerator design, optimization and analysis.

(2) **ACE3P** code suite, with DOE SciDAC and SLAC support, has been benchmarked and used in a wide range of applications in Accelerator Science and Development.

(3) **ACE3P** provides advanced capabilities in its modules **Omega3P, S3P, T3P, Track3P, and Pic3P** that have enabled challenging problems to be solved worldwide.

(4) Computational science R&D enabled under SciDAC and high performance computing are essential to tackling real world problems through simulation.

(5) The **ACE3P** User Community is formed (SLAC hosted the code workshops CW09 [15] and CW10 [16]) to share this resource and experience and we welcome the opportunity to collaborate on projects of common interest.

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