I. Facilities, Equipment, and other Resources

SUNY-Environmental Science and Forestry

Laboratory/Office/Computer

The proposed research will be carried in graduate student research offices located in Jahn Laboratory, which was completed in 1997. Offices are wired for data transmission and access to the Internet, and cabling was upgraded in Summer 2012 to increase bandwidth. Offices house PCs used for routine word processing and data analysis.

The PI’s group operates a 16-processor quad-core 64-bit Opteron QuantumCube from Parallel Quantum Systems with 96 GB RAM and 4 TB of disk space. The following quantum chemistry software is currently installed on this system:

GAMESS, CFOUR, GAUSSIAN09, NWChem 6.5, NBO4.1

The following kinetics software is currently installed on this system:

POLYRATE, GAUSSRATE, MultiWell

Multiple PCs in graduate student research offices run Gaussian03 for Windows, Gaussview4, Spartan, and software for RRKM/Master Equation calculations (UNIMOL, MESMER, Multiwell).

ESF also supports a Linux-based cluster consisting of 21 nodes with 168 processor cores and 3 GB of RAM per core, yielding a peak performance of 1.3 TFLOPS. Both local and networked storage are available to users. Currently there is a combined 5 TB of storage attached. NWChem 6.5 and CMAQ-Hg is available on this cluster.

Large Scale Computing

For projects that exceed local resources, the PI has routinely obtained grants of computer time from NSF-sponsored Teragrid (now XSEDE) resources.

Other Resources

ESF has an electronics technician and support staff for computer hardware and software.

Mississippi State University

Laser Spectroscopy and Plasma Lab at Mississippi State University (MSU) founded by the co-PI consists of four research laboratories, which are equipped with state-of-the-art equipment and available to support the proposed research. Two 700 sq. ft. new laboratories are in the Department of Physics and Astronomy in the College of Arts and Sciences and two labs are located in the Institute for Clean Energy Technology (ICET) within the College of Engineering at MSU.
Major Equipment

Laser diagnostics and spectroscopy, especially CRDS, is a primary component of the co-PI’s research program. The major equipment housed in the co-PI’s four laboratories are: five 4 × 6 ft² optical tables; one recently acquired OPO system (Spectra-Physics, MOPO-HF with PRO-270-10, linewidth < 0.075 cm⁻¹, spectral range 227 nm – 4.3 µm); two sets of Nd:YAG pumped dye laser systems (one with frequency doubling and the other with tripling), covering wavelength from 197 nm to 740 nm; one spectrograph with an EMCCD (Princeton Instrument); one external cavity diode laser (ECDL ) from New Focus; one ECDL from New Port with two gratings and three laser heads at different wavelength; two sets of diode laser drivers (IXL and New Focus); several DFB laser diodes; two free space double-stage optical isolators (1570, 1650 nm); two PMTs covering UV to VIS; one fast NIR photo-receiver; one MIR detector; one double grating monochromator equipped with fiber waveguides; two digital oscilloscopes (Tektronix 410, 460A); two pulse generators; one vacuum-pumped CRDS cell, one vacuum-free flow CRDS cell; one supersonic slit jet CRDS system; ringdown mirrors cover major wavelengths from 226 nm to 1650 nm; self-developed CRDS software; one inductively coupled plasma; one microwave induced plasma system; one set of cold plasma jets; one mass spectrometer (QMS200); one ultra nebulizer; one fiber splicer; one fiber cleaver, one set of fiber fabrication kit; five computers.

Other Resources

ICET is located at 58,000 ft² facilities housing fifteen research laboratories operated by faculty members from different academic departments. ICET has a full machine shop, digital and analog electronics shops, and a high-bay testing facility. These resources will be also available for the proposed research.

Unfunded Collaborations

Unfunded collaborations are described here (see also Letters of Commitment) as specified in the NSF Grant Proposal Guide (II.C.2.d.iv).

Dr. Dibble will work with his ESF colleague Dr. Huiting Mao and her students to incorporate the results of this research into Dr. Mao’s box model and a version of CMAQ-Hg. As Dr. Mao and her students have offices within steps of Dr. Dibble’s office, this collaboration requires no special effort to manage.

Dr. Dibble will work with Dr. Daniel Jacob and his graduate student, Hannah Horowitz, to incorporate the results of this research into the global 3-D GEOS-Chem model. Much of the collaboration will be managed by email and phone/video conference. There will also be opportunities to meet in person at, for example, the Gordon Conference on Atmospheric Chemistry or the International Conference on Mercury as a Global Pollutant.