(SICM)$^2$ Parallel Computing Workshop

### Attendees

**Chemistry**
- Daniel Crawford: PSI, many-body
- Sarom Leang: GAMESS
- Edoardo Apra: DFT, NWChem
- Eduard Valeev: Many-body, MPQC
- Ilya Kaliman: Many-body, QChem
- Gary Trucks: Gaussian
- Bryan Sundahl: TDFT, NWChem, MADNESS
- Lubos Mitas: QMC
- Robert Harrison: NWChem, MADNESS

**Materials**
- Robert DiStasio: Plane wave DFT, Quantum Espresso, QChem
- Jack Deslippe: GW, BerkeleyGW
- Scott Thornton: DFT and GW, misc
- Paul Crozier: Molecular dynamics, LAMMPS
- Markus Eisenbech: Many-body, DCA++

**Computer science**
- Beverley Sanders: SIAL, ACES
- Laximant Kale: Molecular dynamics, Charm++, NAMD, OpenAtom
- Bradford Chamberlain: Languages, Chapel
- Sriram Krishnamoorthy: Global Arrays, NWChem
- Anthony Danalis: DAG-based methods
- P. Sadayappan: Tensors, polyhedral optimizer
- Yonghong Yan: OpenMP
Draft Agenda

Friday 6-9pm SUNYRF Global

6:00-6:05  Welcome

6:05-6:30  Crawford – S2I2M2 vision and status

6:30-9:00pm  Chemistry and Materials – challenges and opportunities

6:30-7:00  Harrison – Workshop objectives, challenges and opportunities

Subsequent presentations to address these questions

• Summary of the science domain
  ◦ Example applications(s) in 2020
  ◦ What drives the frontier? Size, time, sampling, ...
  ◦ How big are the user and developer communities?
  ◦ What types and scale of computing are relevant in 2020
    ▪ Lots of terascale jobs? Petascale? Exascale?

• Computational algorithms
  ◦ E.g., Mesh, FFT, linear algebra, ...
  ◦ Relevant dimensions, memory capacity, floating point intensity, ...
  ◦ How will these change by 2020?

• What languages, parallel programming models, etc., are used in this domain?

• What are your current plans for 2020?

• With regard to sustaining HPC software in your domain
  ◦ What up to 3 success stories exist now?
  ◦ What are the top 3 challenges now?
  ◦ What do you see as the top 3 challenges in 2020?

7:00-9:00  Chemistry materials talks – each talk is 15 minutes

• Trucks – View from Gaussian/industry
• Apra – Gaussian molecular electronic structure
• DiStasio – Plane wave DFT
• Deslippe – GW
• Crozier – Molecular dynamics
• Eisenbach – Many body
• Wrap up and plans for next day
Saturday SUNY Manhattan

9:00:11:40am Computer science – challenges and opportunities

Subsequent presentations to address these questions
• What is your elevator story for the scientists?
  ◦ A little detail behind the elevator story
  ◦ Present and future challenges in HPC
  ◦ Your vision/approach to parallel programming
• With regard to designing and programming HPC codes
  ◦ What up to 3 success stories exist now?
  ◦ What are the top 3 challenges now?
  ◦ What do you see as the top 3 challenges in 2020?
• How should scientists be thinking of a sustainable path forward?
  ◦ How can we drive relevant standards?
  ◦ How can we help enable relevant innovations?
  ◦ What must/can/should we do for ourselves?
• Roles for computer science research, students, and products in the institute?

Each of the following is 20 minutes
• Laximant Kale – Charm++, NAMD, OpenAtom
• Beverley Sanders – SIAL, ACES
• Sriram Krishnamoorthy – Global Arrays, Resilience
• Anthony Danalis – DAG-based composition
• Break
• P. Sadayappan – Tensors, polyhedral optimizer
• Yonghong Yan – OpenMP
• Bradford Chamberlain – Chapel, life, the universe

11:40-11:45 Quick break

11:45-12:00 Mitas – QMC (rescheduled from last night)

11:50-12:45 Discussion as big group
  Objective: Mind meld on objectives and initial path forward for the break out sessions

12:45-1:45 Lunch (box lunch provided)
1:45-3:15  Breakout session 1 (90 minutes)
Attendees will be pre-assigned to sections

Breakout A. Molecules

Breakout B. Materials

Objectives:
• Identify challenges and opportunities
• What do we need to expand participation?
• What do we need to accelerate discovery/innovation?
• Current state of art in science domain
• Science drivers for 2020
• Characteristics of computation in 2020
• Opportunities and road blocks
• Who/what is not in the room?
• What should a sustainable approach aspire to?

3:15-3:30  Break

3:30-5:00  Breakout session 2 (90 minutes)
Attendees will be pre-assigned to sections

Breakout C. Emphasizing productivity

Breakout D. Emphasizing performance

Objectives:
• Identify challenges and opportunities
• What do we need to expand participation?
• What do we need to accelerate discovery/innovation?
• What are absolute must dos?
• What are conservative reliable approaches?
• What are blue sky potentially transformational approaches?
• Who/what is not in the room?
• What should a sustainable approach aspire to?

5:00-5:15  Break

5:15-6:00  Big group (45 minutes)
• Summary presentations and discussion
• Discuss agenda and objectives for Sunday

Sunday SUNY Manhattan
9:00-10:30  Breakout session 3 (90 minutes)
Attendees will be pre-assigned to sections

Breakout E. Education

Breakout F. Community, collaboration, architecture

Objectives:
• What should we be teaching?
• How should we organize?
• How do we maintain our brands and yet develop communally?
• Two-way educational efforts: Can we train domain scientists in just enough software design and computer scientists in just enough science to make serious progress?
• Giving credit for thankless work: how can we ensure that those developing infrastructure are recognized for their efforts?
• Career opportunities: Can developing tools rather than methods yield desirable permanent positions?
• What kind of environment, people, and resources provide the best opportunity for serious collaboration between computational scientists and computer scientists? Can any sort of top-down effort succeed?
• How broadly should our community be defined? Are our software challenges for large-scale computing sufficiently similar that we're part of the same tribe?

10:30-10:45  Break

10:45-11:45  Big-group discussion

11:45-2:00  Working lunch (box lunch provided)