$(SICM)^2$ 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	Real space DFT, PARSEC
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
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
- Mitas – QMC
- DiStasio – Plane wave DFT
- Deslippe – Real space DFT
- 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
- 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

11:40-11:50 *Quick break*

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)*