A numerically exact solver for electron-phonon lattice models in the polaron limit

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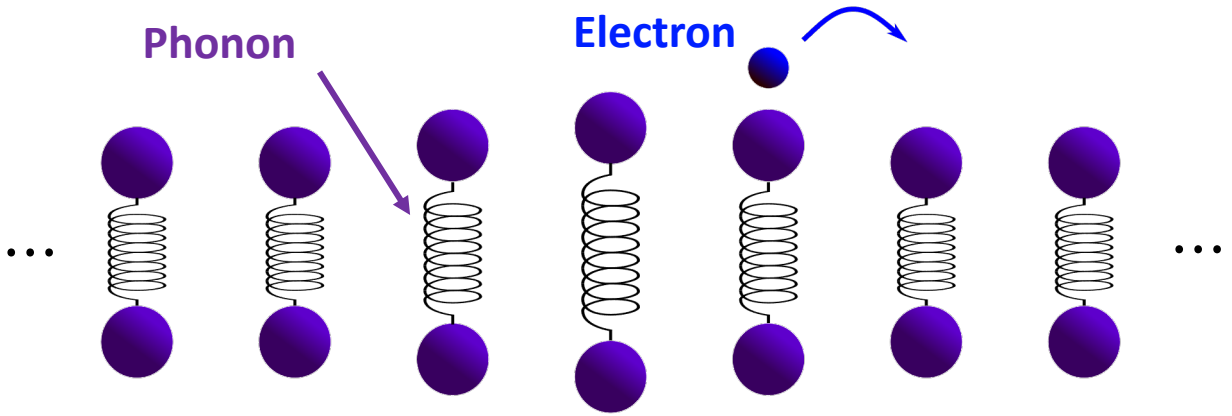
DOE CSGF 4th year talk – 2021 [Virtual] Annual Program Review

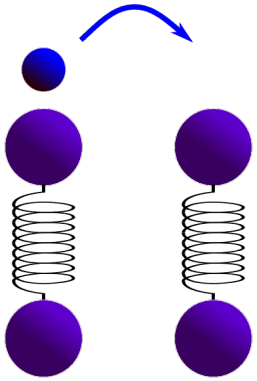
Overview

- **What are we doing?**
  - Solving for the “single particle response” of the system: i.e., what happens when you inject an electron into an otherwise empty lattice?
  - We propose a method that is systematically exact (methodologically unconstrained)
- **Why are we doing it?**
  - Solve many model physical problems of interest (theorist’s curiosity)
  - Eventually use to probe real materials, such as Holstein/Peierls couplings in organic crystals
  - Develop a user-friendly, HPC-ready API for eventual open-sourced deployment
- **What am I presenting today?**
  - Brief introduction to the electron-phonon problem and [theoretical] single-particle spectroscopy
  - Description of our method, the Generalized Green’s function Cluster Expansion (GGCE)
  - Demonstration of the method through selected results
  - API highlight, and future usage of HPC

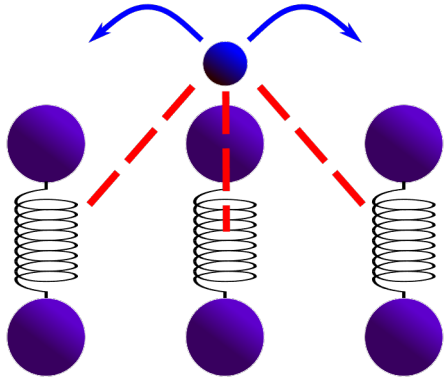
What is the electron-phonon system?



Infinite (1D) lattice



The electron can "hop" from site to site



The electron can create and destroy phonons locally

The system has some energy (Hamiltonian):

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\Omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q}} g(\mathbf{k},\mathbf{q}) c_{\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}} (b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}})$$

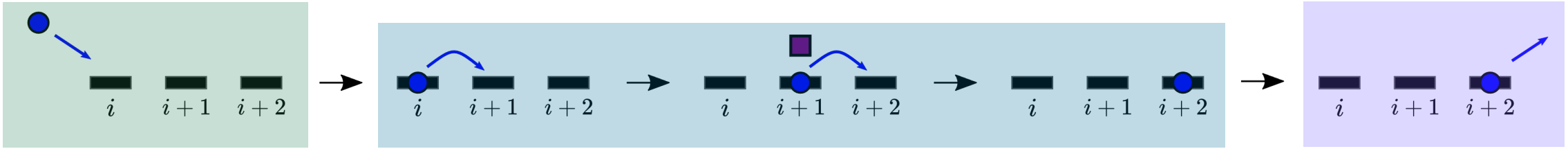
- **Electron energy given by free particle lattice dispersion:** $\varepsilon_k = -2t\cos(ka)$
  - **"For each electron on the lattice, index it's momentum quantum number and assign it the appropriate energy"**
- **Phonon energy given by phonon dispersion**
  - **Essentially the same idea as the electrons**
  - **We approximate a "dispersionless" (constant) phonon energy, Ω**
- **Interaction term defined by linear coupling and vertex**
  - **Renders the model non-analytic**

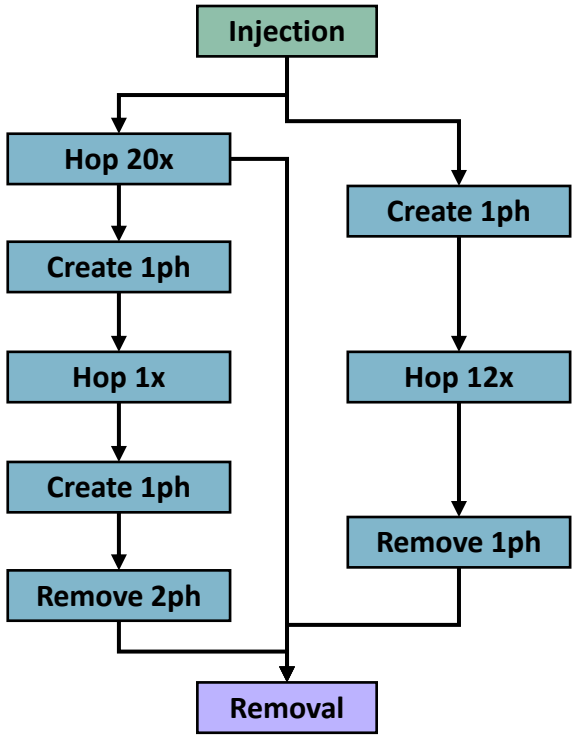
Measuring single-particle spectra

(1) An electron is injected (removed) from the lattice

(2) The electron propagates through the system, creating and annihilating phonons

(3) After eliminating all phonons, the electron is removed from the lattice





There are many ways for the electron to propagate, eventually ending up somewhere with no phonons

$$G(\mathbf{k},t) = -i\Theta(t)\langle 0|c_{\mathbf{k}}e^{-itH}c_{\mathbf{k}}^{\dagger}|0\rangle$$

Such a process is given by the retarded Green's function; it sums *all* ways in which this process is possible! Quantum mechanics assigns the "weight" to each of these "paths".

$$G(\mathbf{k},\omega) = \langle 0|c_{\mathbf{k}}G(\omega)c_{\mathbf{k}}^{\dagger}|0\rangle$$
$$G(\omega) = [\omega - H + i\eta]^{-1}$$

It is useful to represent the Green's function in frequency-space, since its imaginary part is a spectral function/density of states, and is *measurable*

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\,G(\mathbf{k},\omega)$$

Connection to experiment

Angle-resolved photo-emission spectroscopy (ARPES)

Damascelli, Hussain & Shen.
Rev. Mod. Phys. **75**, 473 (2003)

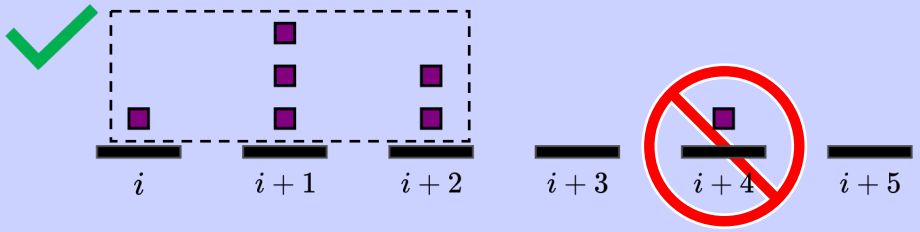
Methodology overview

Exact analytic approach

There are in fact an *infinite* number of ways for the electron to propagate on the lattice

$$G(k,\omega) = \langle 0|c_k G(\omega) c_k^\dagger|0\rangle$$

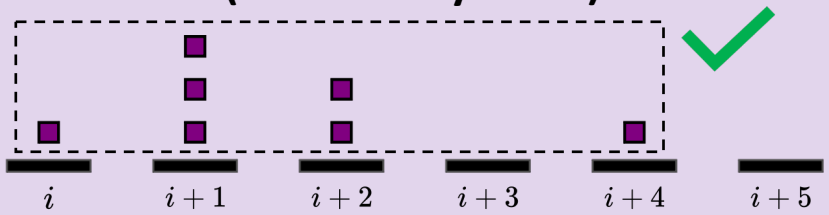
Momentum Average Method (approximate)



- Leverages ansatz that phonons come in clouds
- Polarons
- Restricts cloud *extent* (M) and *phonon number* (N)
- No restriction on electron
- Can run on your laptop

Berciu, Phys. Rev. Lett. **97**, 036402 (2006)

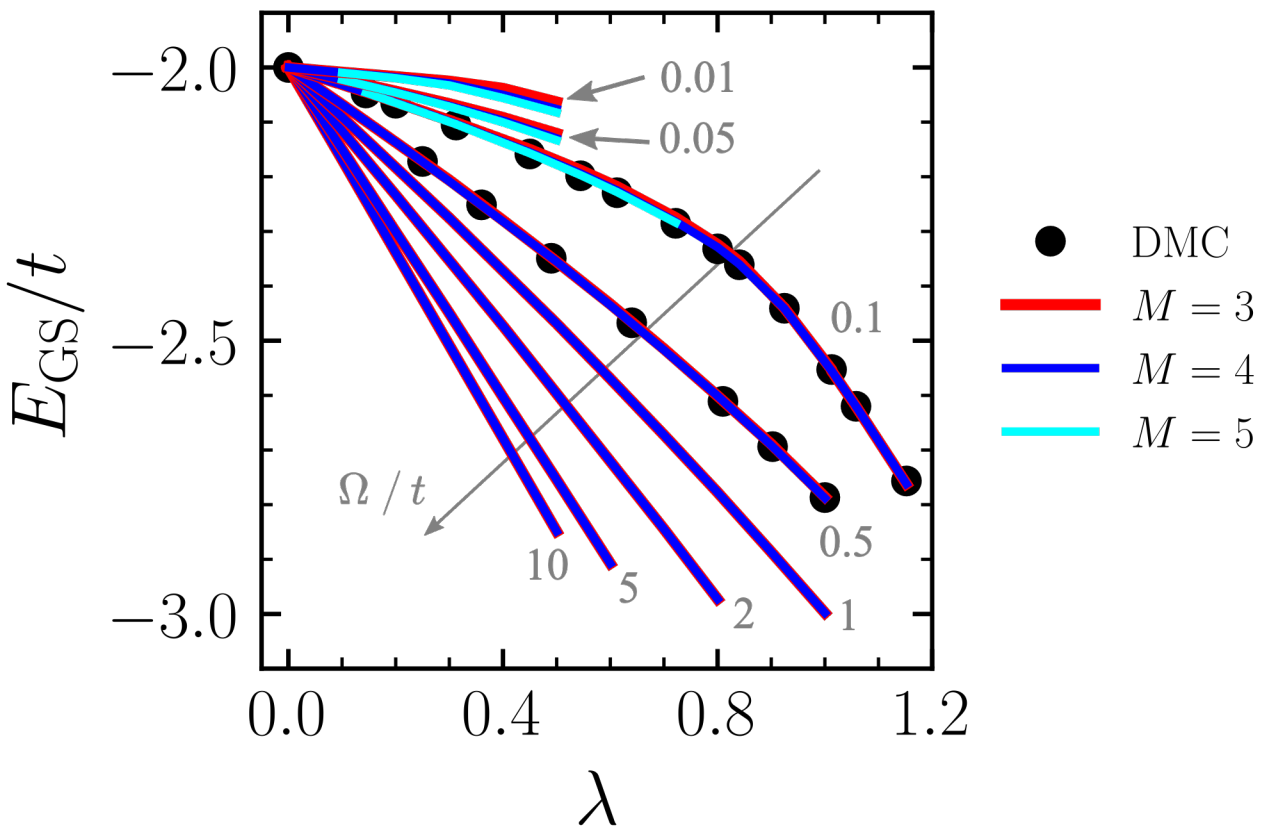
Generalize Green's function Cluster Expansion (numerically exact)



- Generalizes the Momentum Average family to systematically converge with respect to M and N
- Seamlessly handles multi-phonon mode models (e.g. Holstein+Peierls), as well as finite-temperature
- Can easily be extended to more than one dimension, multi-carrier band, and multi-carrier (e.g. bipolaron) models
- User-friendly API
- HPC-ready firepower (PETSc+MUMPS currently)
- Scaling is a combinatorics problem: "balls in bins" (exponential, but empirically tractable)
- User has direct control over desired "level of theory"
- For every k,w-point, M and N value, the task at hand is to solve a huge system of linear equations

MRC, Reichman & Sous, *accepted* Phys. Rev. B.

Holstein model ground state results



A. Macridin, Ph. D. Thesis, Rijksuniversiteit Groningen (2003)
MRC, Reichman & Sous, *accepted* Phys. Rev. B.

$$V = \alpha \sum_i c_i^\dagger c_i (b_i^\dagger + b_i)$$

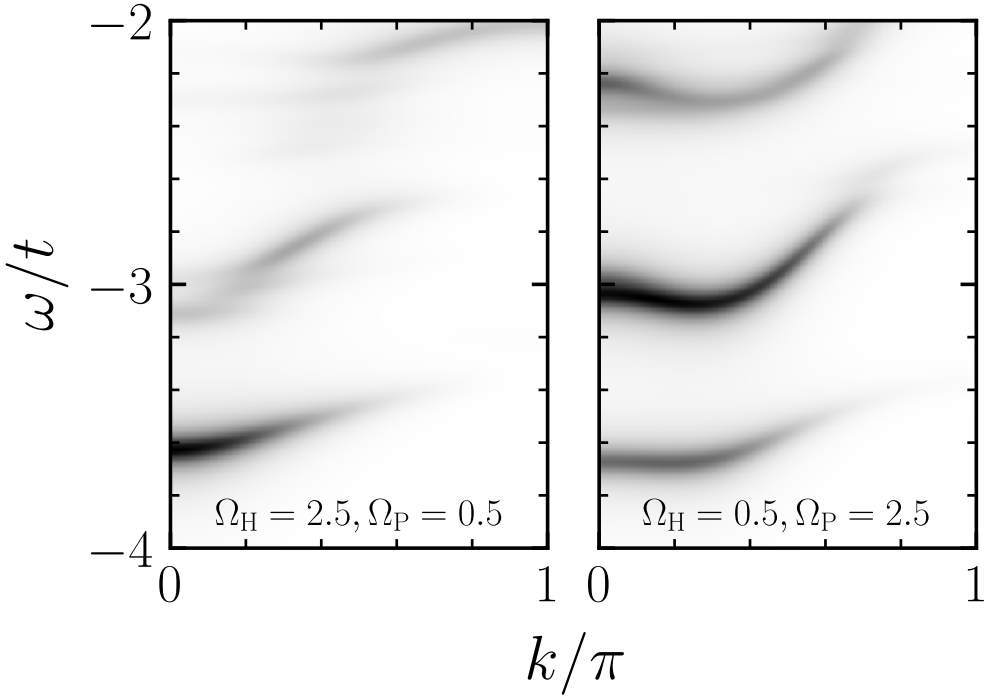
Holstein coupling: local phonon creation and annihilation occurs without electron movement

- Our results agree perfectly with Diagrammatic Monte Carlo (DMC), a popular numerically exact technique
- With some effort, we can obtain converged intermediate-coupling results in the extreme adiabatic limit

Holstein+Peierls model spectra

$$V = \alpha_{\mathrm{H}} \sum_i c_i^\dagger c_i (b_i^\dagger + b_i) + \alpha_{\mathrm{P}} \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)(d_i^\dagger + d_i - d_{i+1}^\dagger - d_{i+1})$$

Holstein + Peierls coupling: local and non-local phonon creation is allowed, mechanisms compete

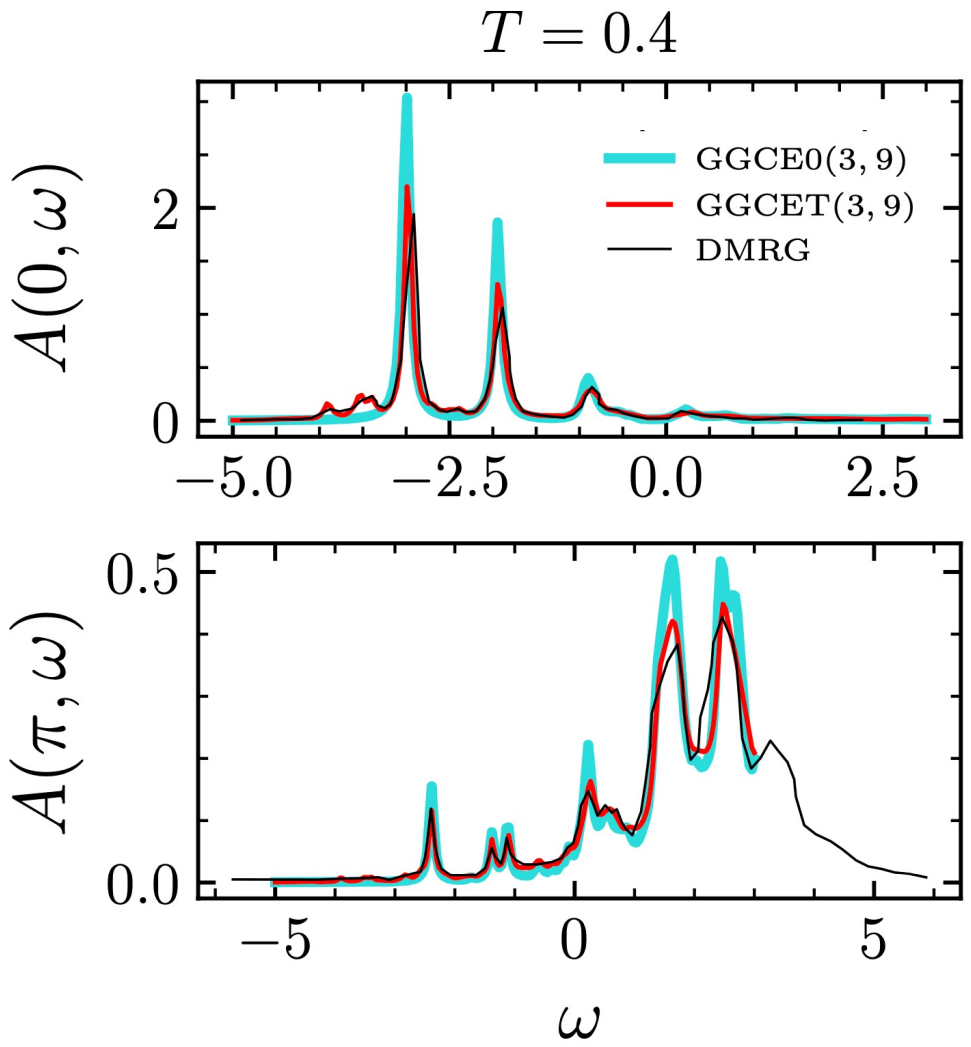


- Holstein (local) + Peierls (non-local) coupling
- Real materials have multiple couplings mechanisms
  - Equal dimensionless coupling strengths, various phonon frequencies
- We can handle this seamlessly in the GGCE method

MRC, Reichman & Sous, *accepted* PRB

Finite-temperature Holstein model spectra

- "Thermofield double"
  - Maps a finite T, n-phonon mode model onto a zero T, 2n-phonon mode model
- Ground state is no longer a polaron!
  - Corresponds to a polaron ejecting >0 phonon quanta



Jansen, Bonča, Heidrich-Meisner, PRB **102**, 165155 (2020)

Takahashi and Umezawa, Int. J. Mod. Phys. B **10**, 1755 (1996).
Suzuki, J. Phys. Soc. Japan **54**, 4483 (1985).

Results in summary

- **We present a variety of results to demonstrate the scope of our method**
- **So far, "boilerplate" HPC (threads, local memory) has been sufficient**
  - "Single model" results scale *like* "N choose M" (+nontrivial system dependence)
  - Primary workhorse for aforementioned work was the NERSC Cori Haswell architecture: maxed out at around a 200 node simulation
- **However, future problems scale worse, we'll require massively parallel solvers to do this (MPI, distributed)**
  - Single model, finite temperature scales like "N choose 2M"
  - Dual-phonon mode model at 0 temperature scales like "N choose 2M"
  - Dual-phonon mode model at finite temperature scales like "N choose 4M"
  - Current implementation is PETSc+MUMPS parallel sparse solvers
    - Each (k,w) point can be parallel across many nodes

API highlight

```
from ggce.model import Model
model = Model("my_model", "info", log_file=None)
model.set_parameters(hopping=1.0, lattice_constant=1.0, temperature=0.4)
model.add_coupling("Holstein", Omega=0.5, M=3, N=9, dimensionless_coupling=3.0)
model.add_coupling("Peierls", Omega=0.8, M=2, N=4, dimensionless_coupling=2.0)
```

Models are constructed easily in just a few lines of code

```
from ggce.executors.serial import SerialDenseExecutor
executor = SerialDenseExecutor(model)
executor.prime()
A_kw = executor.spectrum(k_grid, w_grid, broadening)
```

Suite of executors which call various backends to solve linear system (numpy dense e.g. MKL, scipy sparse)

```
from ggce.executors.petsc4py.parallel import ParallelSparseExecutorMUMPS
from mpi4py import MPI
# Run with `mpiexec -np <N> python3 script.py`
executor = ParallelSparseExecutorMUMPS(model, mpi_comm=MPI.COMM_WORLD)
executor.prime()
A_kw = executor.spectrum(k_grid, w_grid, broadening)
if MPI.COMM_WORLD.Get_rank() == 0:
    # Do things with spectra
```

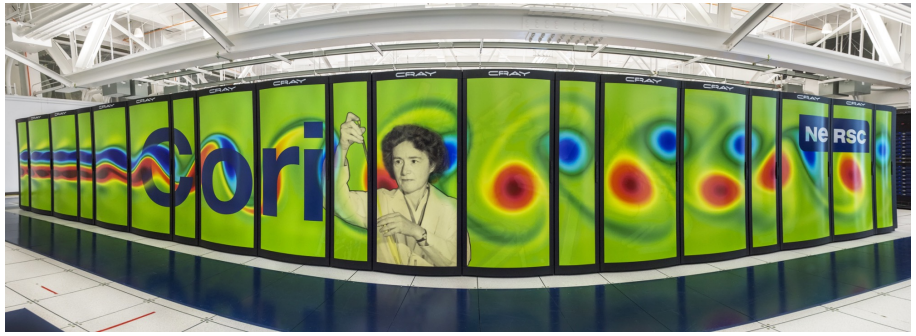
MPI-enabled, PETSc + MUMPS direct sparse solver is essentially HPC-ready

Stepan Fomichev at UBC (Berciu Group)

We have generalized the Momentum Average family of methods to the numerically exact limit whilst allowing the user to choose their desired level of theory. We have used this method to probe the adiabatic limit, compute exact results, and have many more future plans for it!

Acknowledgements

- CSGF coordinators for making our annual conference happen
- Coworkers and advisors
  - David Reichman, Columbia Chemistry
  - John Sous, Columbia Physics
  - Andy Millis, Columbia Physics
  - Mona Berciu, UBC Physics
  - Stepan Fomichev, UBC Physics
- Institutional support, funding & resources
  - DOE CSGF
  - Columbia University
  - NERSC



Thank you! Questions?