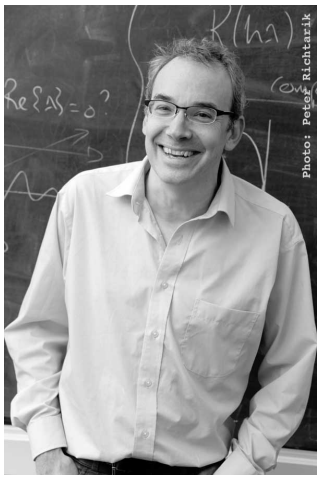
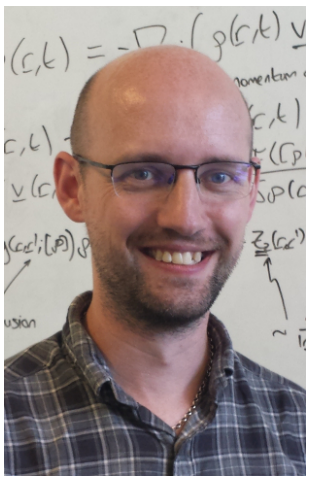
School of Mathematics Groups



Ben Leimkuler

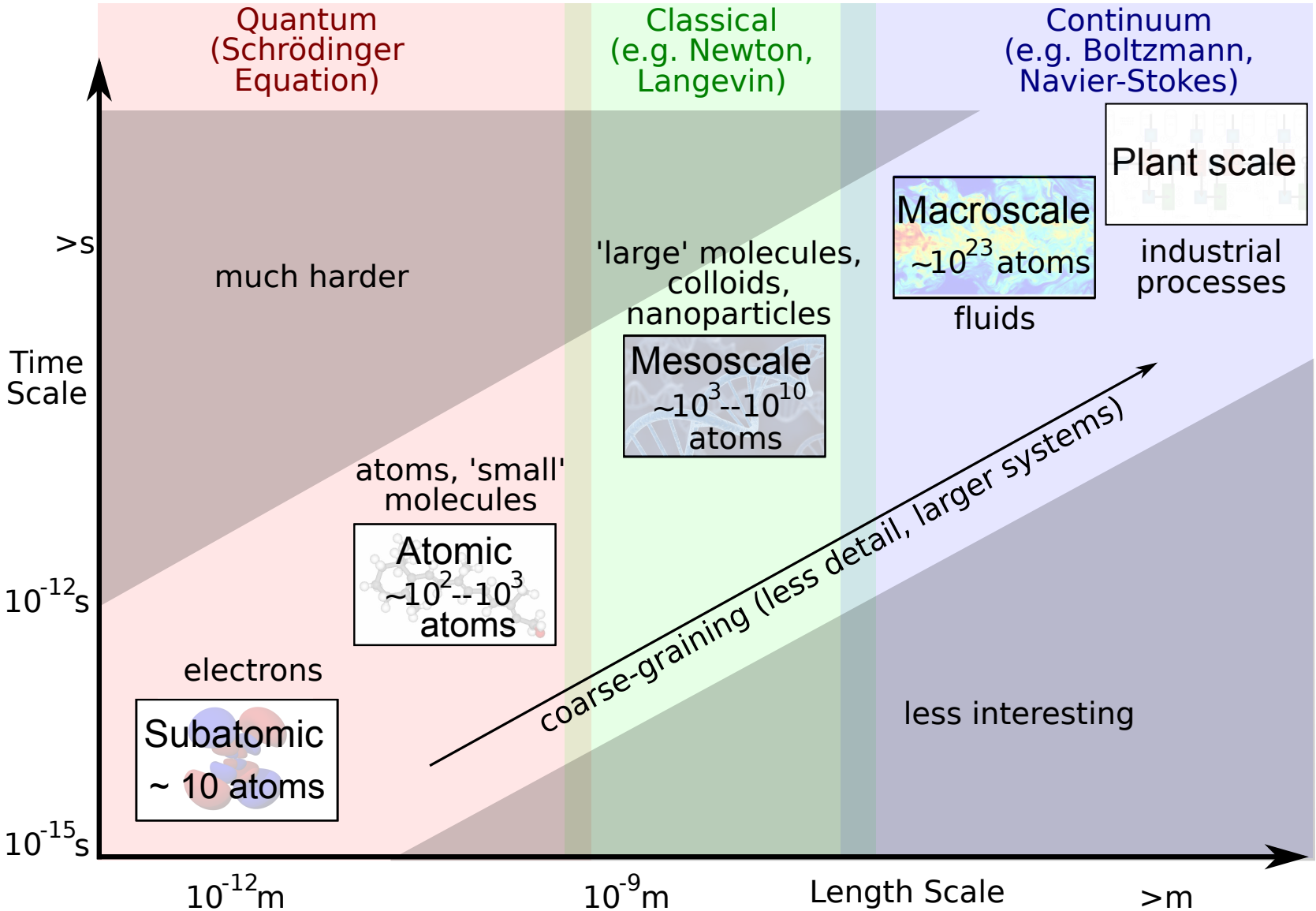
Max Ruffert

Kostas Zygalakis



Ben Goddard

Physical Areas of Interest



Scientific Areas of Interest

- Modelling:
  'The development of a mathematical representation of a physical (biological, chemical, economic, data, . . .) situation.'
  - Quantum
  - Classical
  - Deterministic
  - Stochastic
  - ODEs, PDEs, SDEs, Integro-PDEs

Scientific Areas of Interest

- Modelling:
  'The development of a mathematical representation of a physical (biological, chemical, economic, data, ...) situation.'
  - Quantum
  - Classical
  - Deterministic
  - Stochastic
  - ODEs, PDEs, SDEs, Integro-PDEs
- Numerical Analysis:
  'The design and analysis of techniques to give approximate but accurate solutions to hard problems.'
  - Algorithm design and development
  - Rates of convergence
  - Propagation of errors
  - Numerical stability and well-posedness
  - Why your algorithm fails/is spectacularly good in 'special' cases

Scientific Areas of Interest

- Software Development:
  Some existing projects:
  - ExTASY: Extensible Tools for Advanced Sampling and Analysis
    Novel MD calculations to provide order-of-magnitude improvements in sampling.
  - MD.M: Molecular Dynamics for MATLAB
    Accessible Langevin/Brownian dynamics simulations, in conjunction with Ben L's book.
  - 2DChebClass
    MATLAB pseudospectral scheme for the solution of stiff, non-local, non-linear PDEs.
  - Superadiabatic quantum molecular dynamics
    MATLAB solution of dynamics through avoided crossings.
  - Implementation of novel algorithms in standard packages such as NAMD, LAMMPS, Gromacs

Scientific Areas of Interest

- Interdisciplinary Research
  Currently have collaborations with (at least):
  - Physicists
  - Chemists
  - Biologists
  - Engineers
  - Informaticians
  - Data scientists

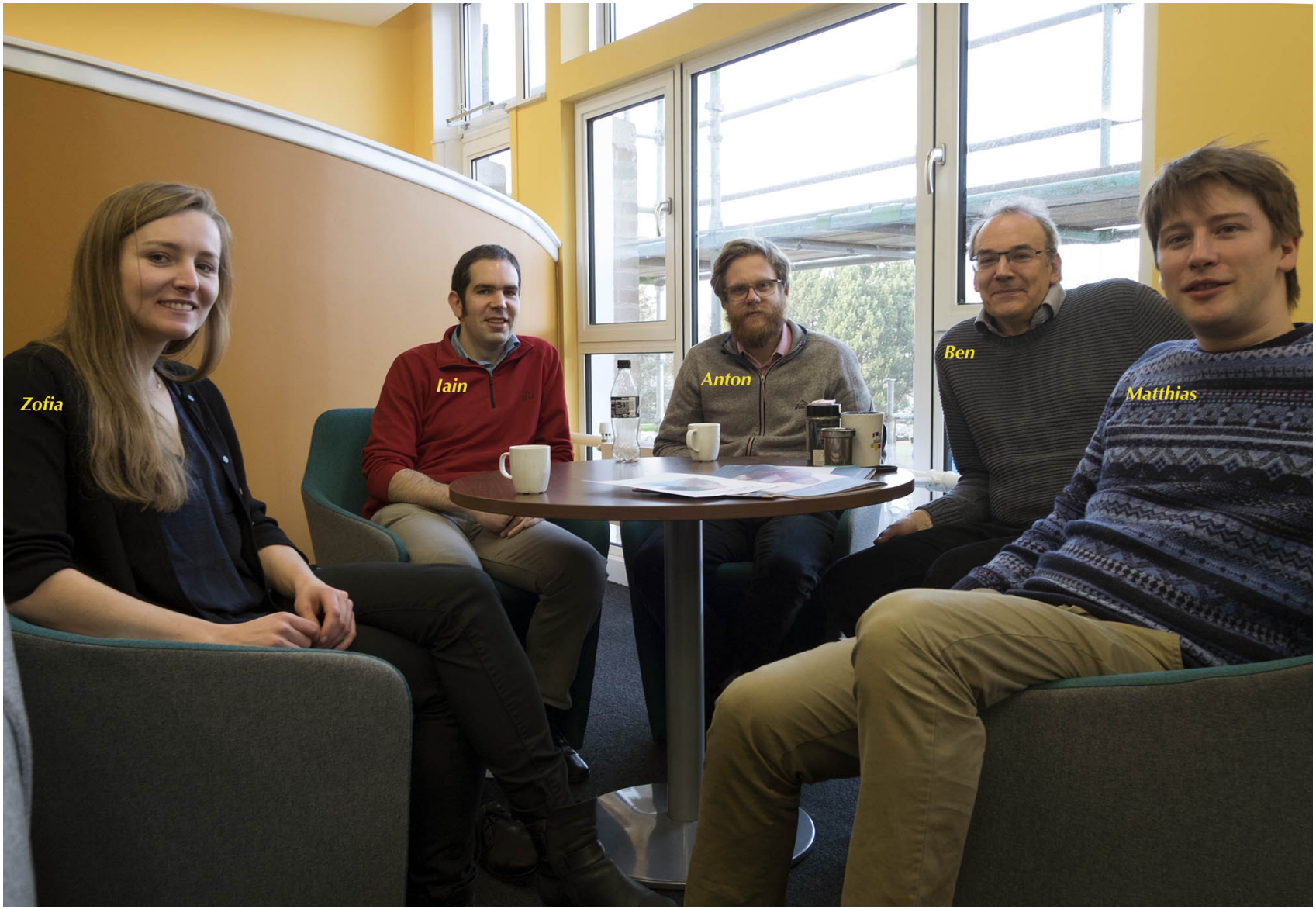
  Keen to have more!

MIGSAA

The Maxwell Institute Graduate School in Analysis and its Applications.

- 12 students per year
- 2 more years of intake
- Currently have 2 MIGSAA students working in MD-related areas (and many more in Applied Maths generally)
- Theme is very broadly-interpreted
- Very happy to have interdisciplinary co-supervision
- Good opportunity to kick-start a collaboration

Leimkuhler Group



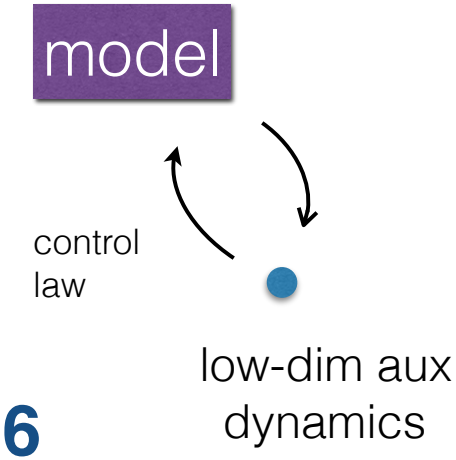
Leimkuhler Group

Variety of work on formulation and stochastic numerical methods for MD simulation in classical biomolecular and mesoscale regimes, including thermostats, barostats, dissipative particle dynamics, Brownian/Langevin dynamics

Current/Recent projects

- **Langevin numerical method**
- **Constant temperature and pressure MD**
- **Adaptive thermostats for nonequilibrium MD**
- **Geodesic integrator for constrained dynamics**
- **Continuous tempering (multiple temperature) strategies**
- **Ensemble quasi-Newton/preconditioned dynamics**
- **Isokinetic stochastic methods for multiple timestepping (100fs stepsizes for MD!)**

Leimkuhler Group



Adaptive Alternatives to DPD

PAdL **L. & Shang, J. Comput. Phys., 2016**

$$\mathrm{d}\mathbf{q} = \mathbf{M}^{-1}\mathbf{p}\mathrm{d}t$$

$$\mathrm{d}\mathbf{p} = \mathbf{F}(\mathbf{q},t)\mathrm{d}t - \xi\boldsymbol{\Gamma}(\mathbf{q})\mathbf{M}^{-1}\mathbf{p}\mathrm{d}t + \sigma\boldsymbol{\Sigma}(\mathbf{q})\mathrm{d}\mathbf{W}$$

$$\mathrm{d}\xi = G(\mathbf{q},\mathbf{p})\mathrm{d}t$$

"Adaptive variant of DPD"

Submitted: **Assessing numerical methods for molecular and particle simulation**

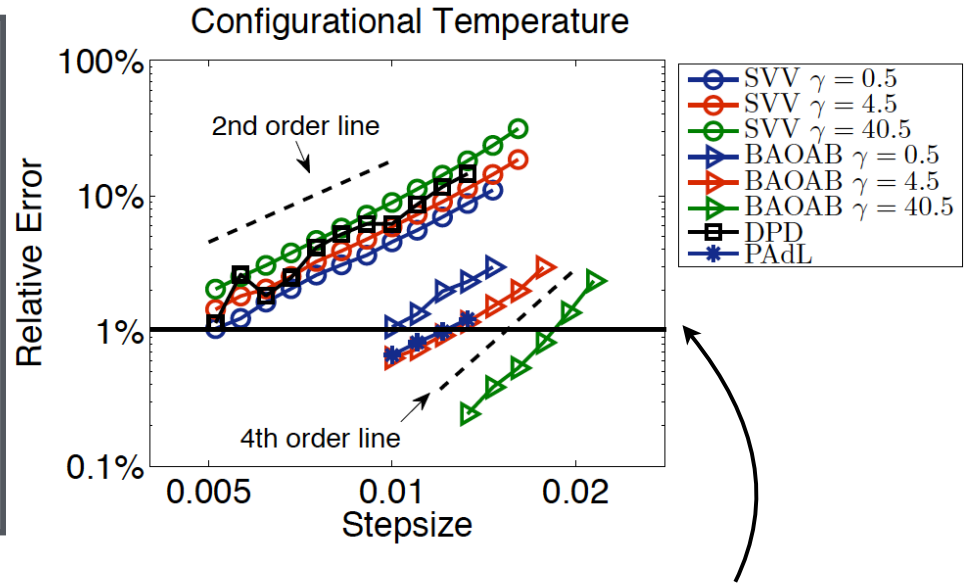
w. **X. Shang (Brown)** and **M. Kroeger (ETH)**

PAdL compared to other schemes for sheared polymer melts

Leimkuhler Group

FENE type Polymer Melts

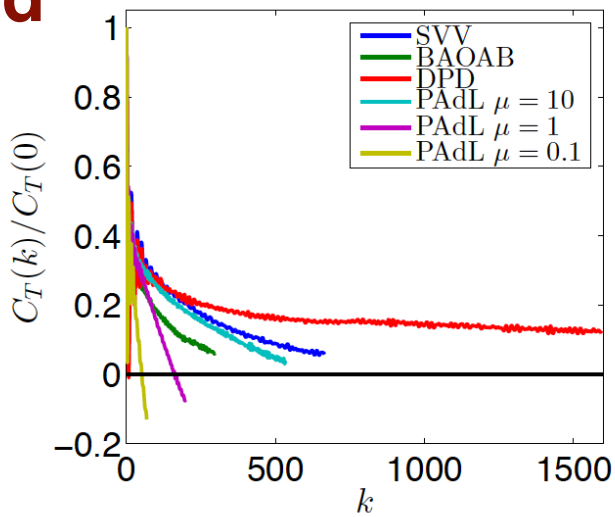
PAdL is typically very accurate for configuration dependent quantities (functions of position)

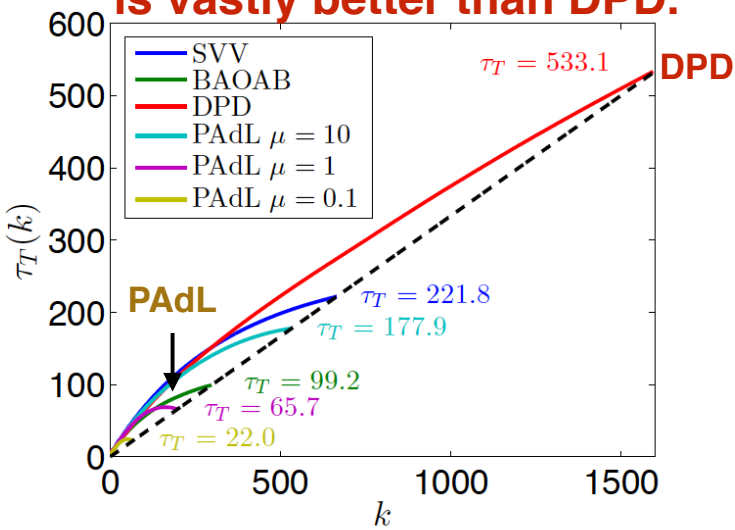


PAdL simulation cost to ach. fixed accuracy is vastly better than DPD.

Much more rapid convergence to equilibrium

v. autocorr. fun.





Zygalakis Group

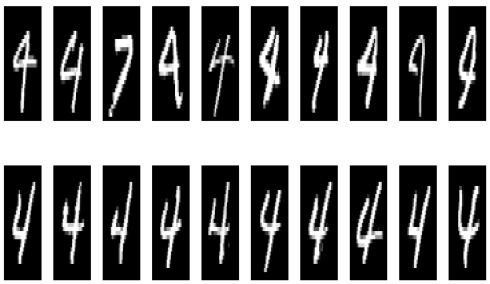
Kostas Zygalakis

Numerical Analysis of SDEs

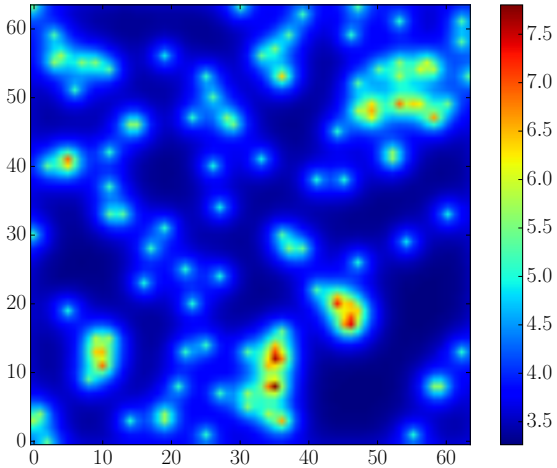
$$dX_t = \nabla \log \pi(X_t) + \sqrt{2} dW_t$$

- Specific type of behaviour as $t \to \infty$ (ergodicity)
- How to discretise such equations? Design and analysis of numerical methods capable of capturing the long time behaviour

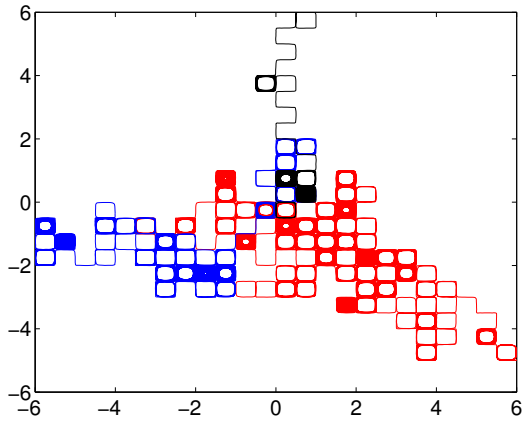
Applications



(a) Machine Learning

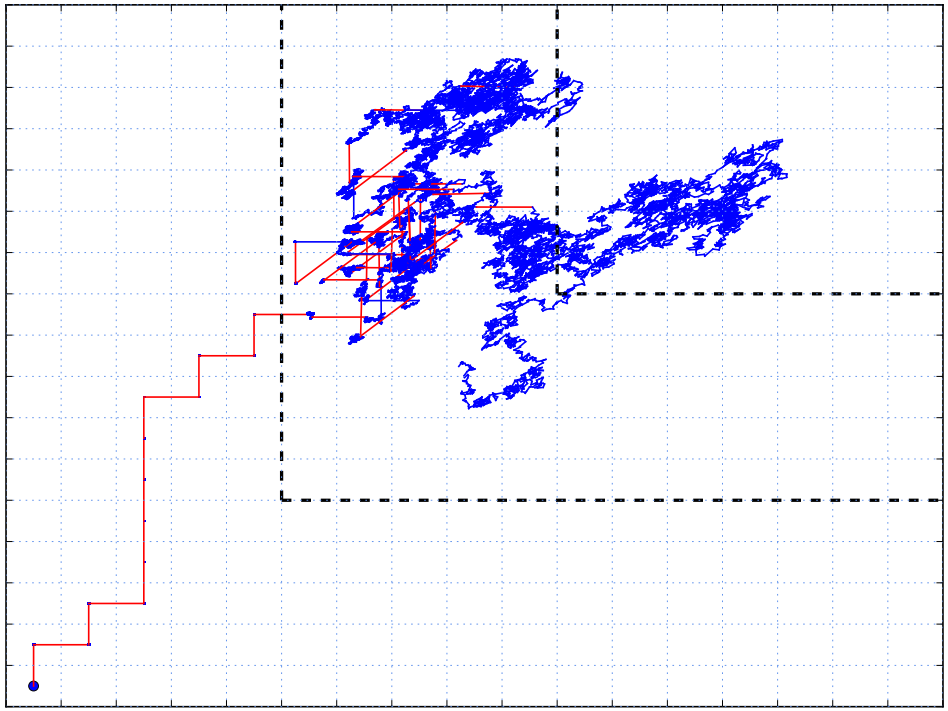


(b) Spatial Statistics

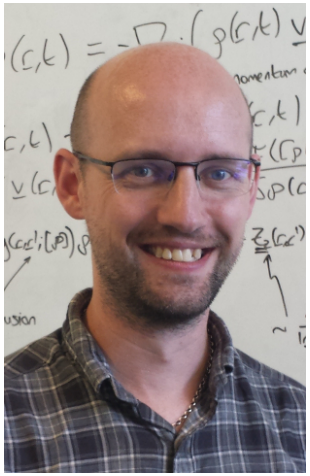


(c) Turbulent Diffusion

Hybrid modelling of stochastic chemical kinetics



Goddard Group



Ben Goddard

Miguel Duran Olivencia

Tim Hurst

Rory Mills

Goddard Group

Modelling, analysis and numerics for a wide range of systems including electronic structure theory, quantum MD and soft matter/complex fluids.

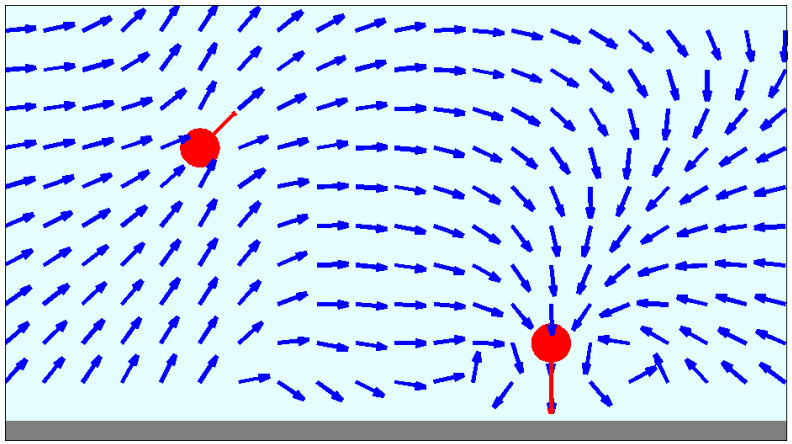
Current projects:

- Statistical mechanics for:
  - soft matter
  - granular media
  - biological systems
- Free energy approximations
- Langevin dynamics, especially with hydrodynamic interactions
- Pseudospectral methods numerical schemes
- Quantum molecular dynamics with avoided crossings

Goddard Group: Dynamical Density Functional Theory

Statistical mechanics for complex fluids.

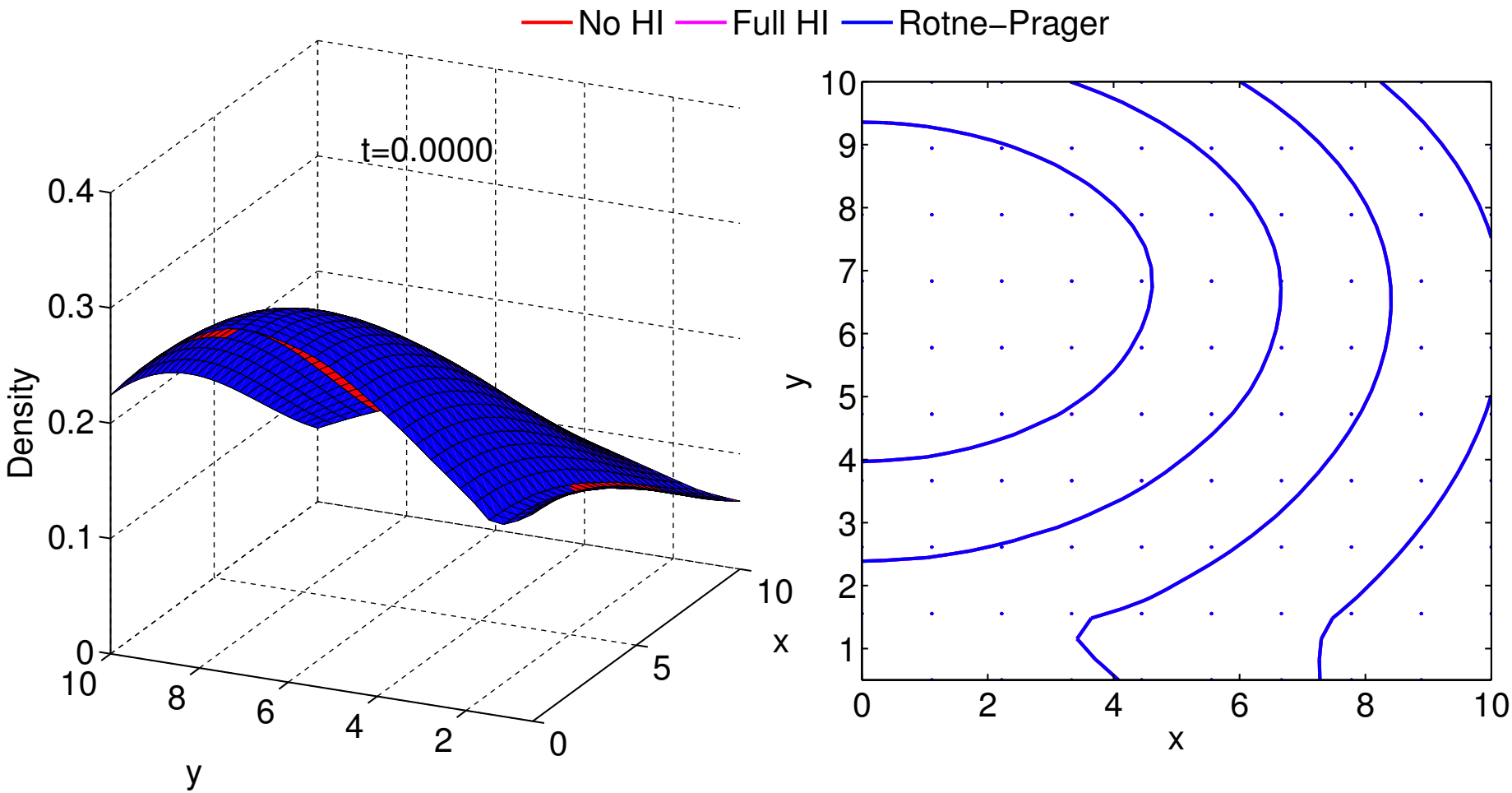
Especially interested in hydrodynamic interactions.



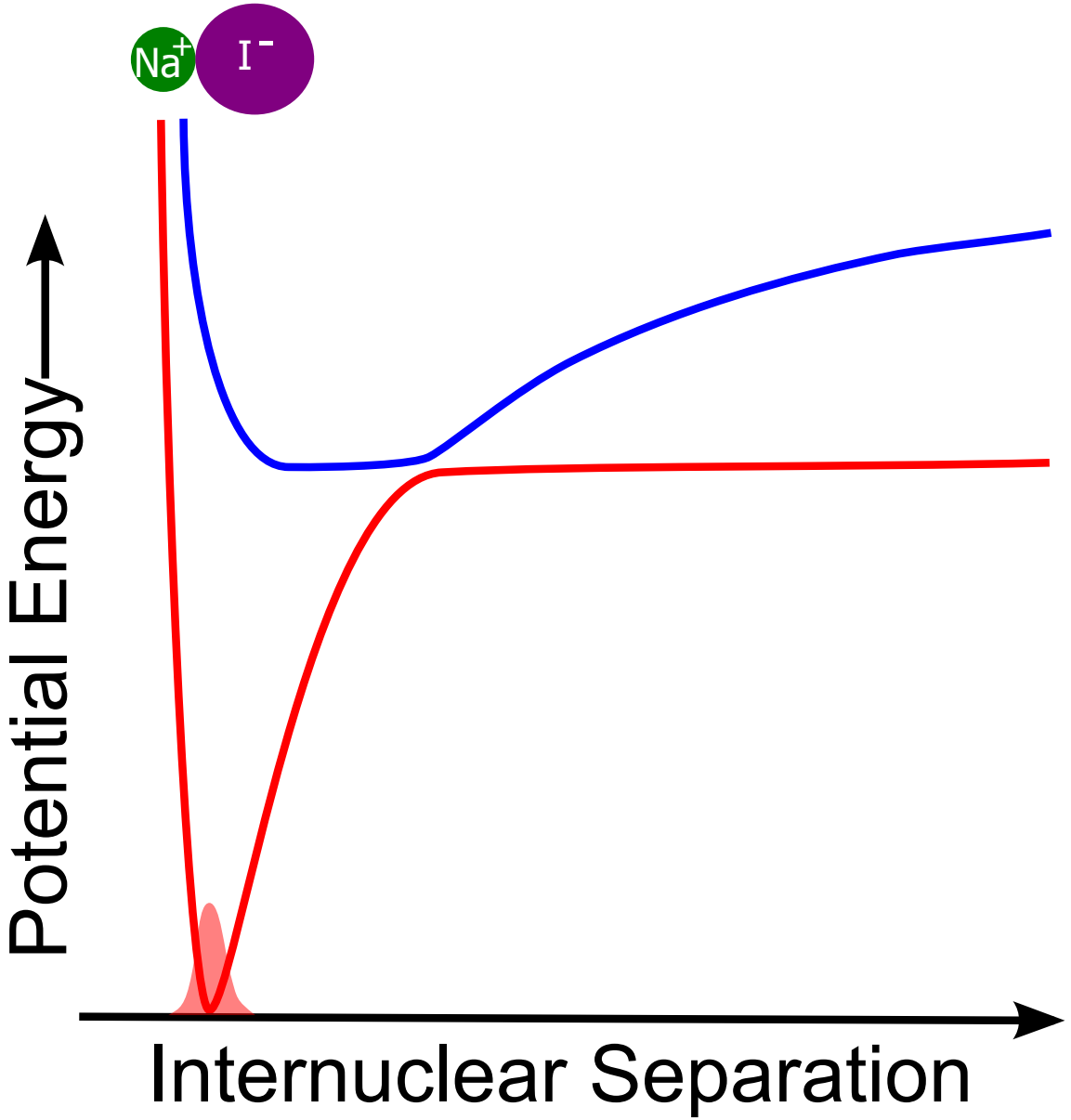
$$\partial_t \rho(\mathbf{r},t) = \frac{D_0}{k_B T}\left[\rho(\mathbf{r},t)\mathbf{W}_0(\mathbf{r},t)\boldsymbol{\nabla}_{\mathbf{r}}\frac{\delta\mathcal{F}[\rho]}{\delta\rho(\mathbf{r},t)}\right.$$
$$+\int \mathrm{d}\mathbf{r}'\rho(\mathbf{r},t)\rho(\mathbf{r}',t)g([\rho];\mathbf{r},\mathbf{r}')\mathbf{W}_{11}(\mathbf{r},\mathbf{r}')\boldsymbol{\nabla}_{\mathbf{r}}\frac{\delta\mathcal{F}[\rho]}{\delta\rho(\mathbf{r},t)}$$
$$\left.+\int \mathrm{d}\mathbf{r}'\rho(\mathbf{r},t)\rho(\mathbf{r}',t)g([\rho];\mathbf{r},\mathbf{r}')\mathbf{W}_{12}(\mathbf{r},\mathbf{r}')\boldsymbol{\nabla}_{\mathbf{r}'}\frac{\delta\mathcal{F}[\rho]}{\delta\rho(\mathbf{r}',t)}\right]$$

With S. Kalliadasis (Imperial), Y. Kevrekidis (Princeton), G. Pavliotis (Imperial), D. Sibley (Loughborough), ...

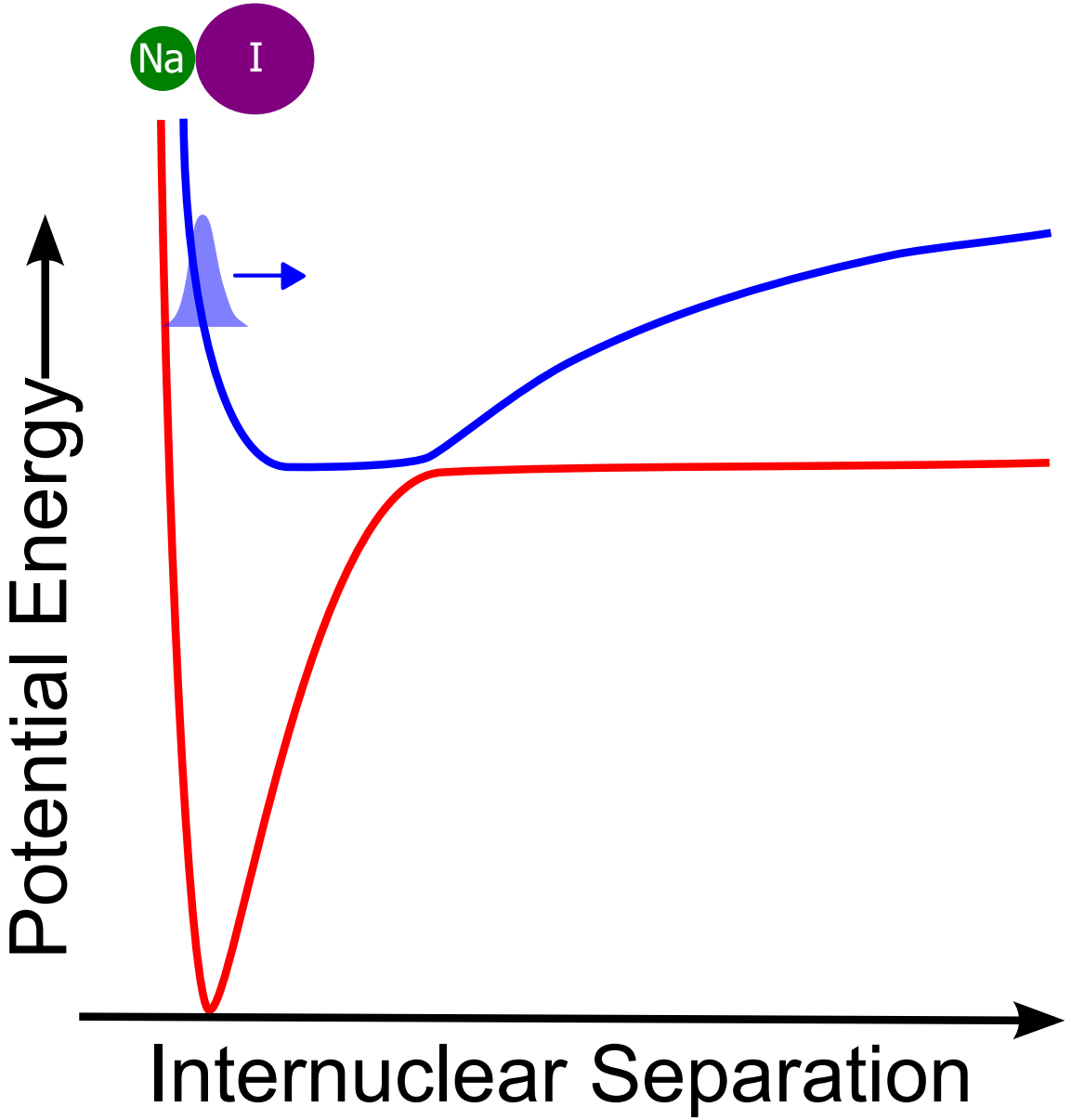
Goddard Group: Dynamical Density Functional Theory

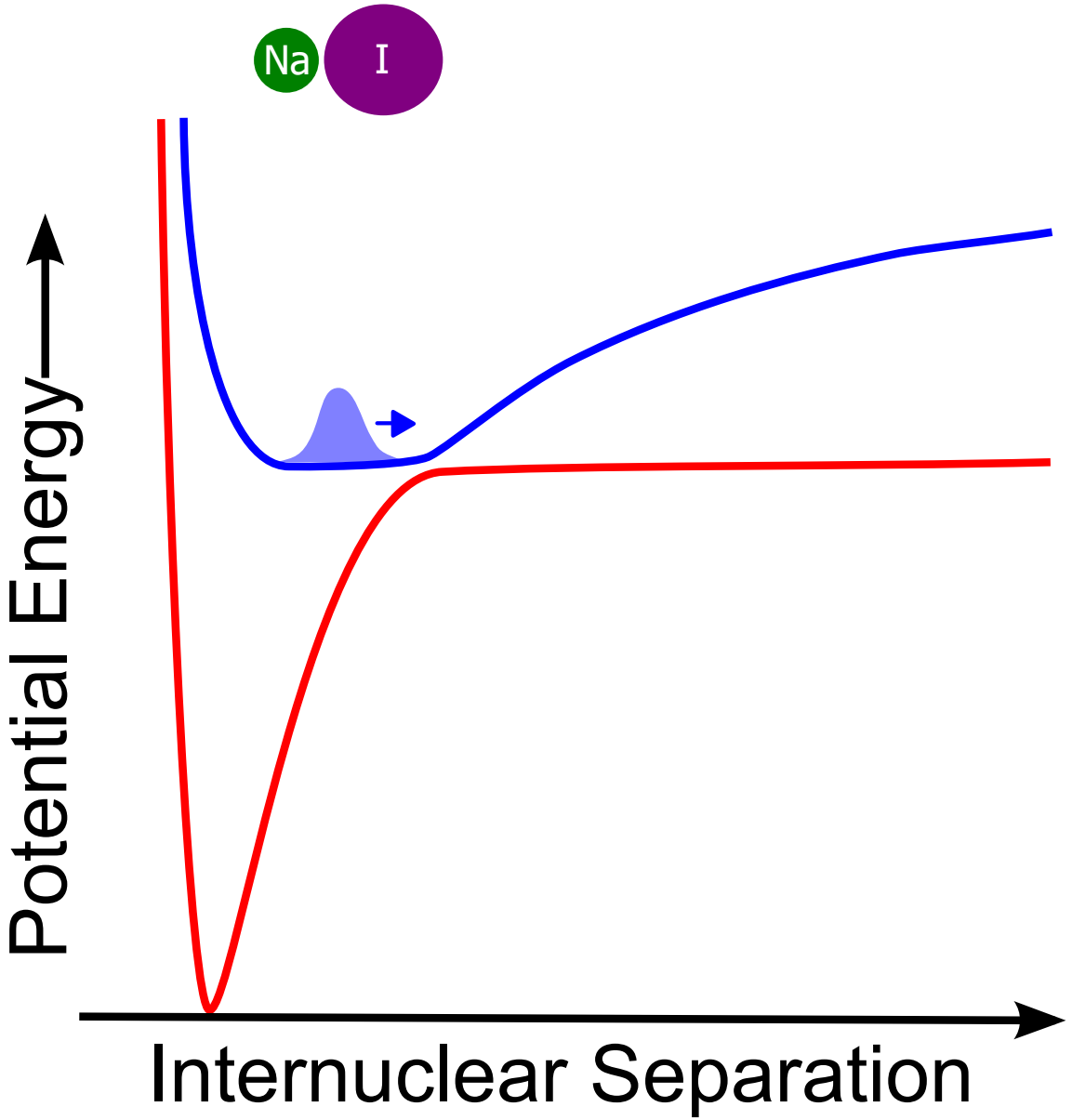


Goddard Group: Quantum MD

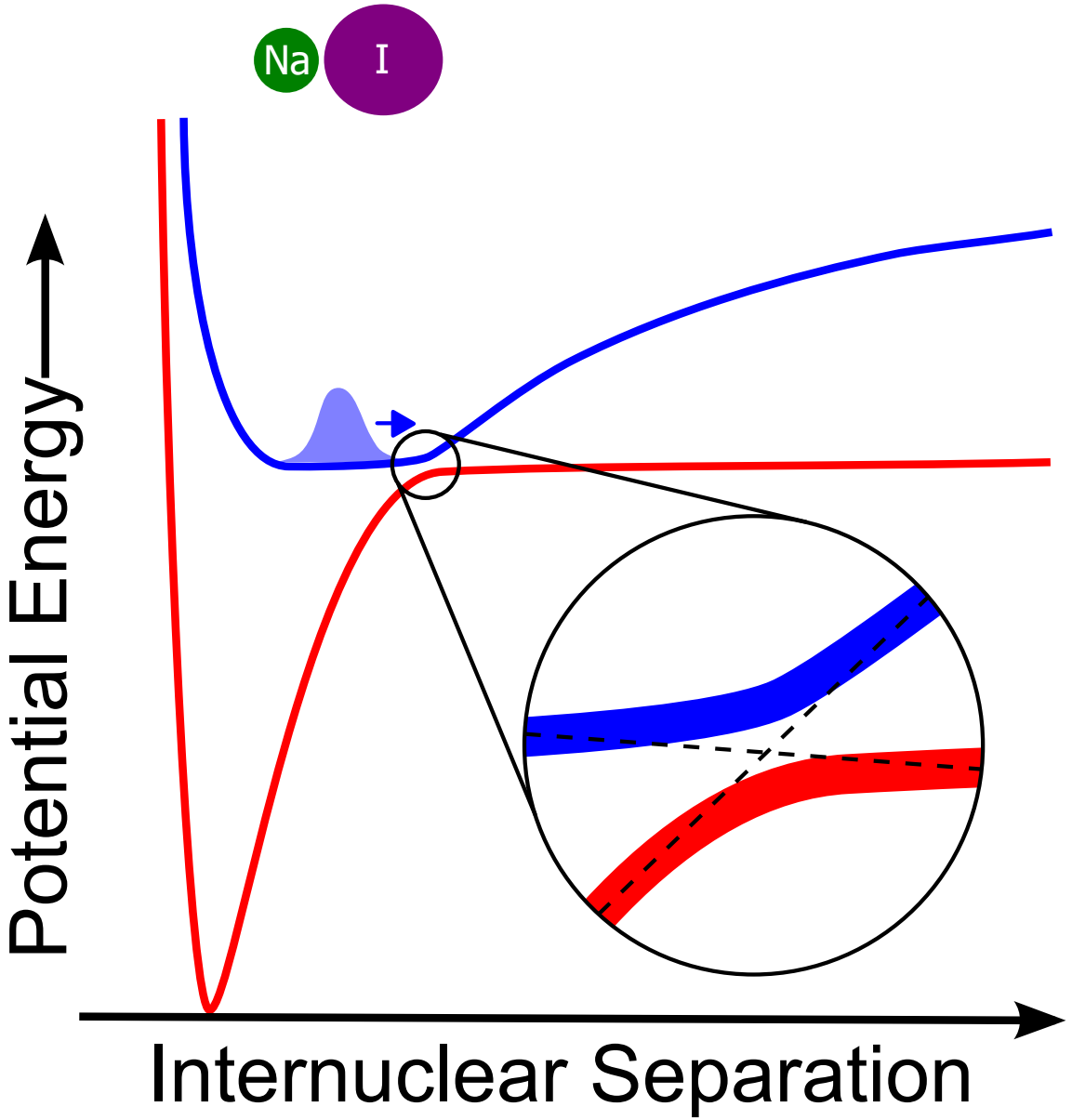


Goddard Group: Quantum MD

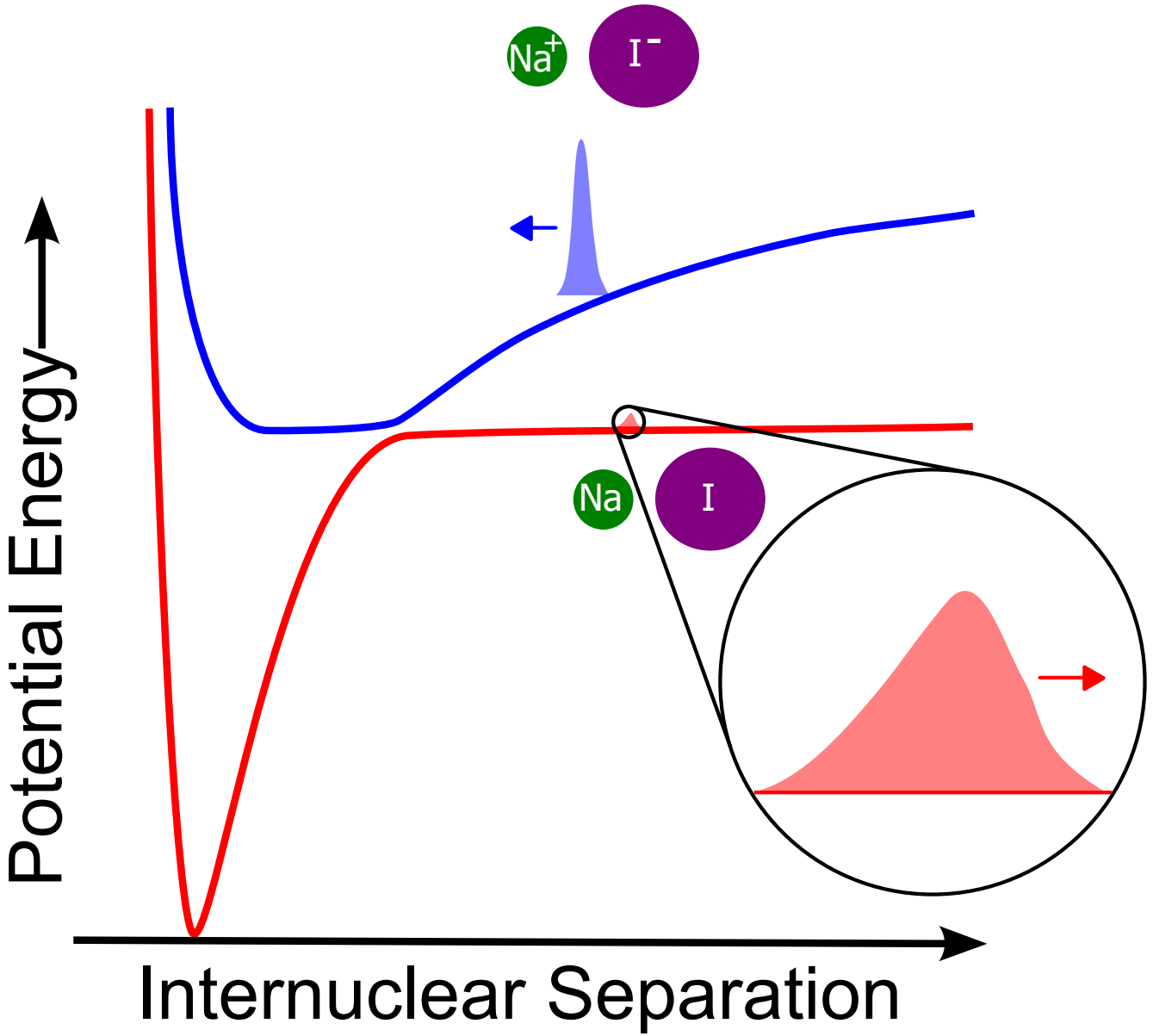



Na
I
Potential Energy
Internuclear Separation

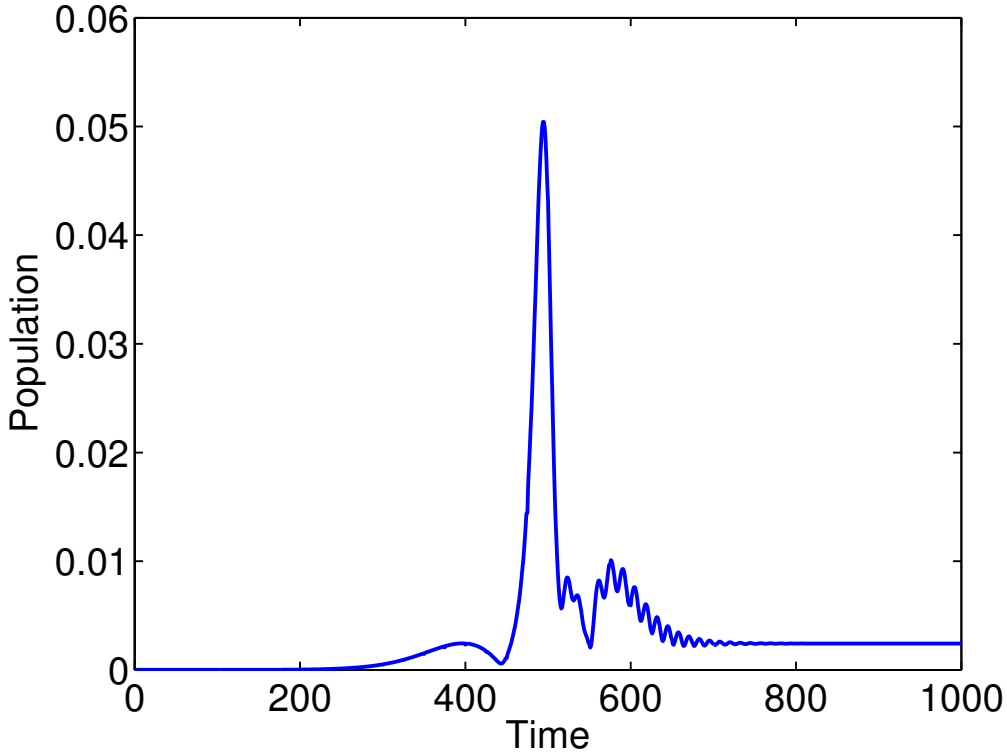
Goddard Group: Quantum MD



Goddard Group: Quantum MD



Goddard Group: Quantum MD

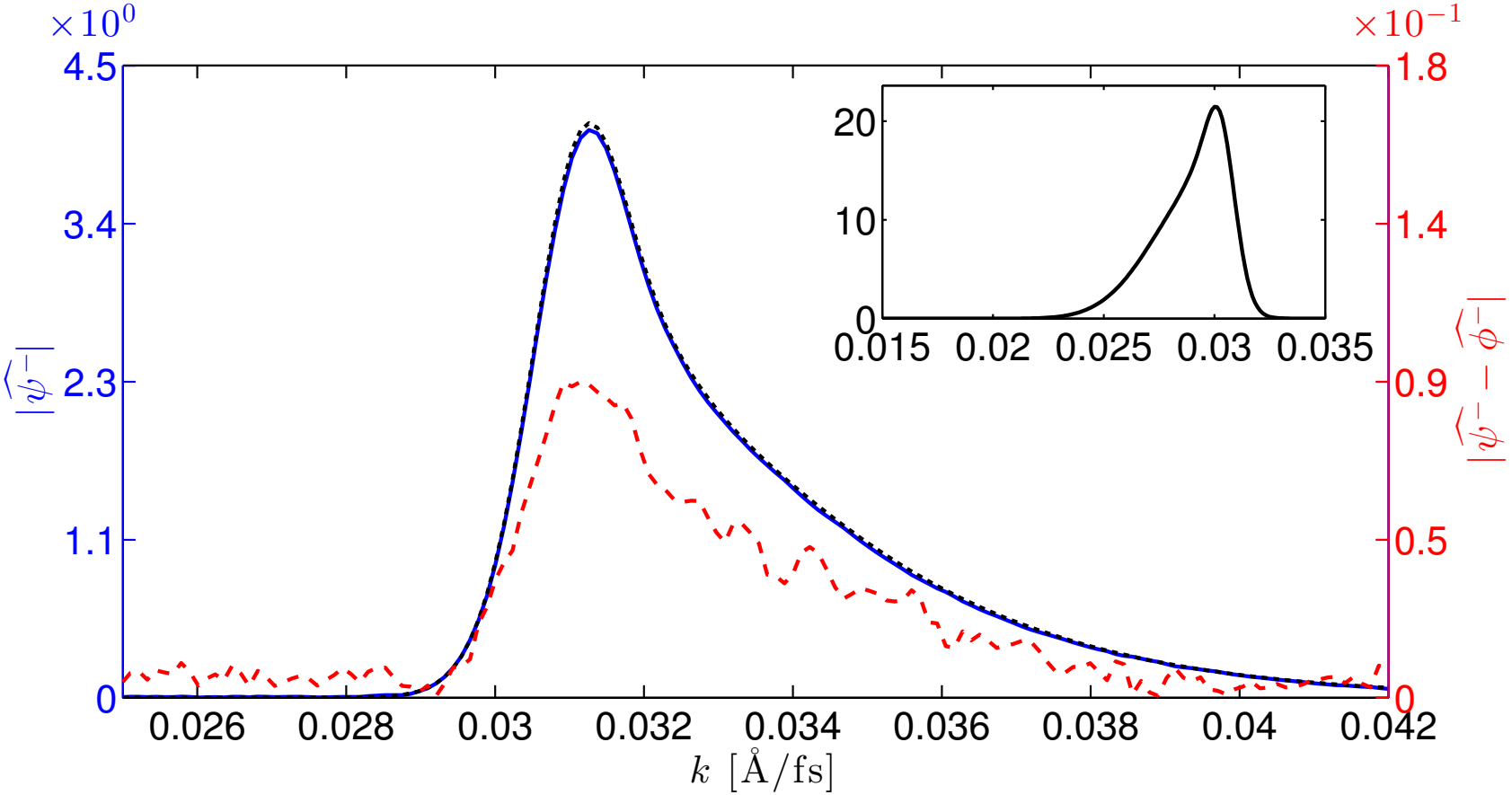


$$\widehat{\psi_n^-}^{\varepsilon}(k,t) \approx \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}t\hat{H}^-}\,\frac{\eta^*+k}{2|\eta^*|}\,\mathrm{e}^{-\frac{\tau_c}{2\delta\epsilon}|k-\eta^*|}\,\mathrm{e}^{-\mathrm{i}\frac{\tau_r}{2\delta\epsilon}(k-\eta^*)}\,\widehat{\phi}^{\varepsilon}(\eta^*)\chi_{k^2>4\delta}$$

Only requires 1-level dynamics and adiabatic PES.

With V. Betz (Darmstadt), U. Manthe (Bielefeld), S. Teufel (Tübingen).

Goddard Group: Quantum MD



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