FabSim

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Computational research is tricky

- We want to do work of “excellent” quality.
- Chart out problems we’ve never tackled before.
- Do computations of unprecedented size and complexity.
- Using state-of-the-art, high quality research production codes.

The reality

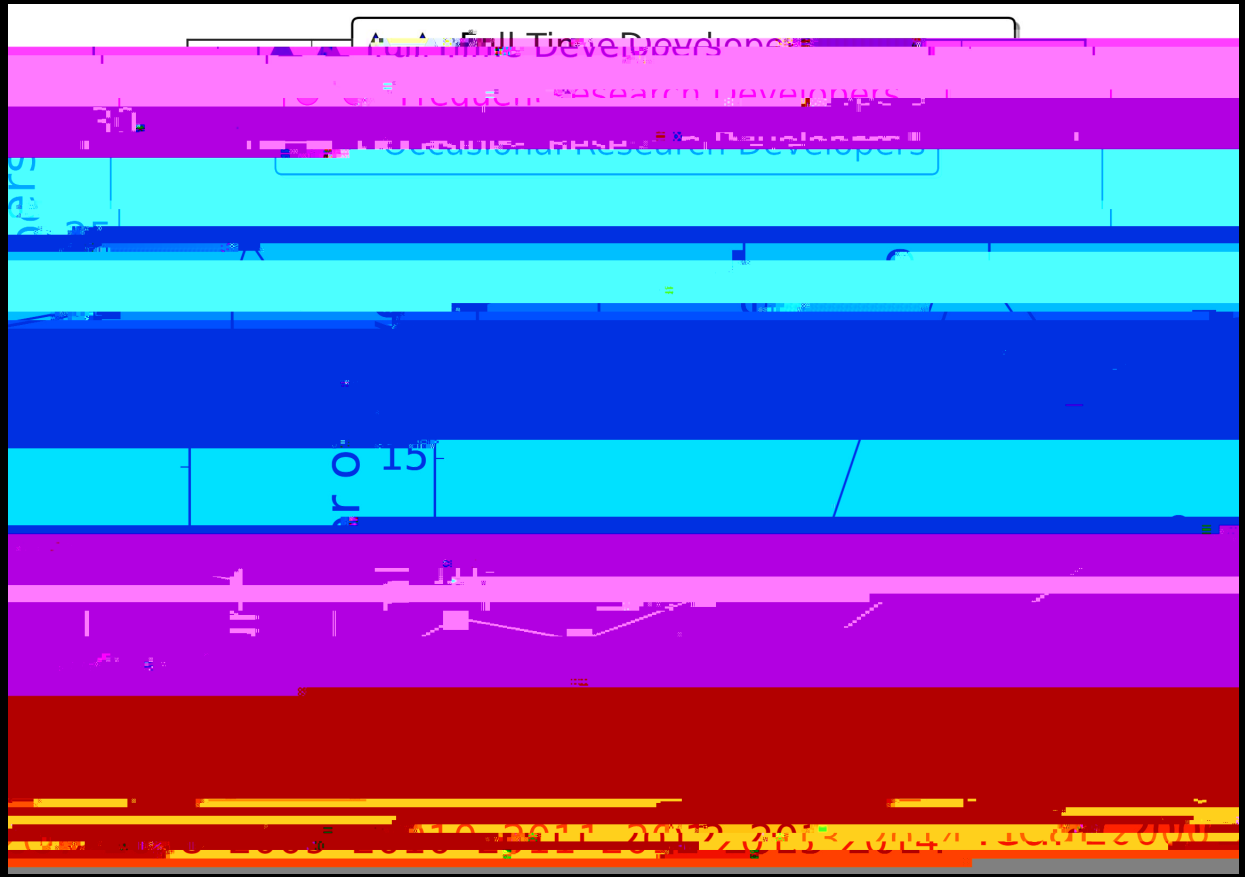
- Projects of limited size, limited duration.
- PhD-ware, *Titanic*-ware.
- Hofstadter’s law.
  - “It always takes longer than you expect, even when

Why do we as academics suck so much, while industry frequently does pull it off to create something solid?

The curious case of academic software

ESPResSo

(major CFD code developed in Germany)

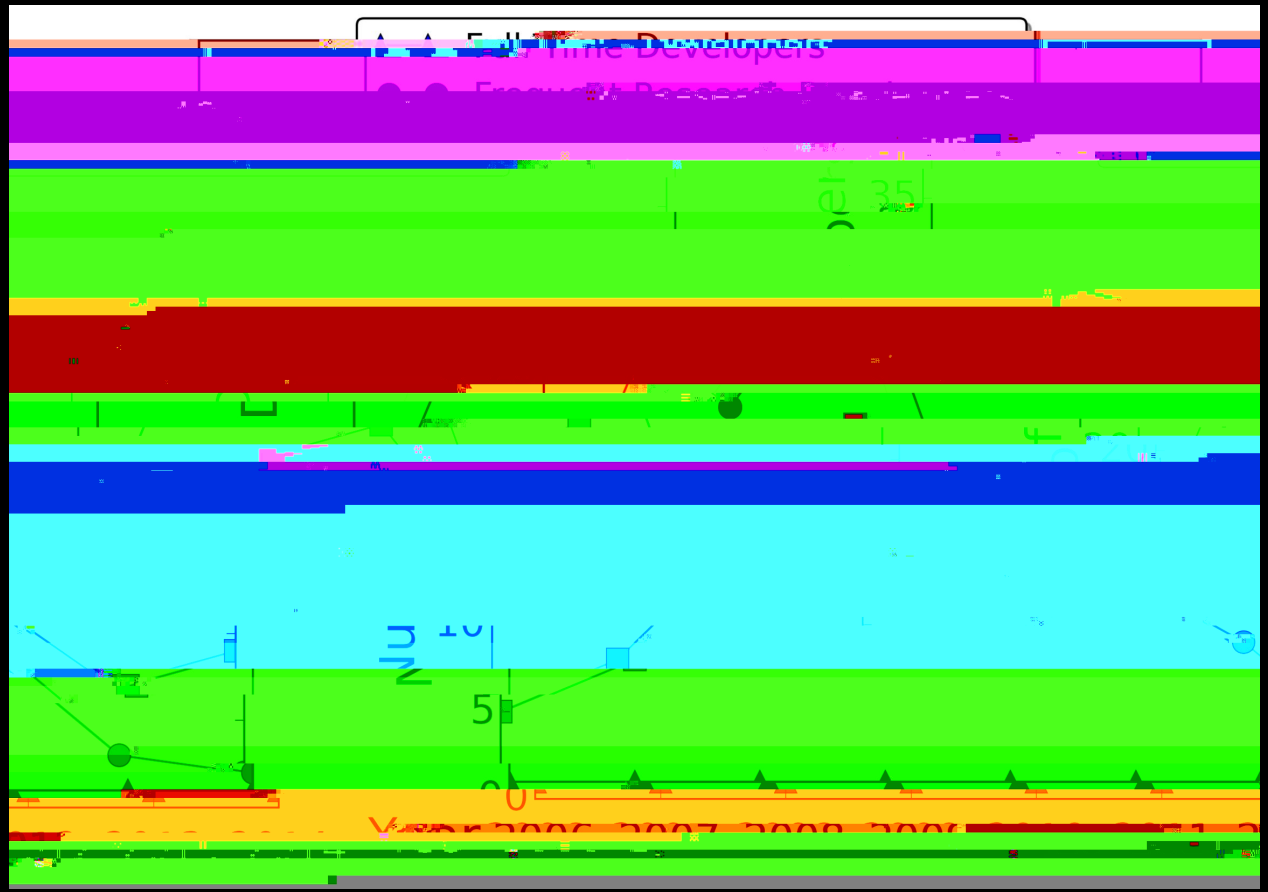


Groen et al., arXiv:1506.05272

The curious case of academic software

Fluidity

(major CFD code developed in the UK)

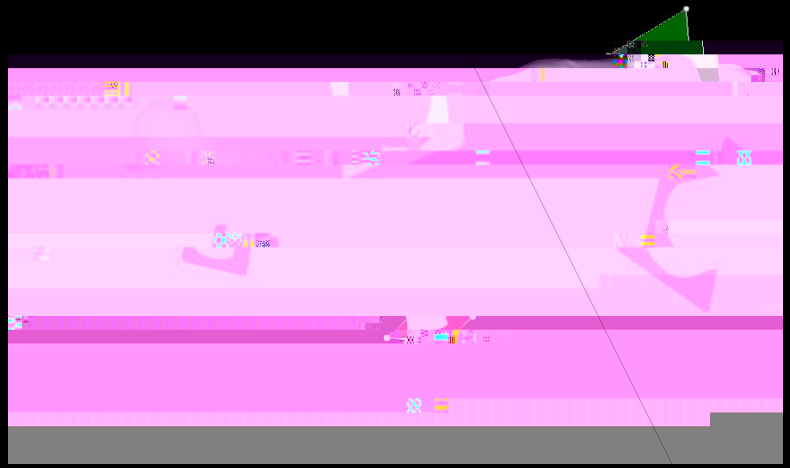


Big data

FabSim: aiming to mitigate Small Effort

- Save time.
- Automate frequently used patterns in computational research.
- Provide quick one-liners to use patterns, or composite ones.
- Prevent double-work, by curating data automatically.
- Make software for the user-developer, not the end-user.

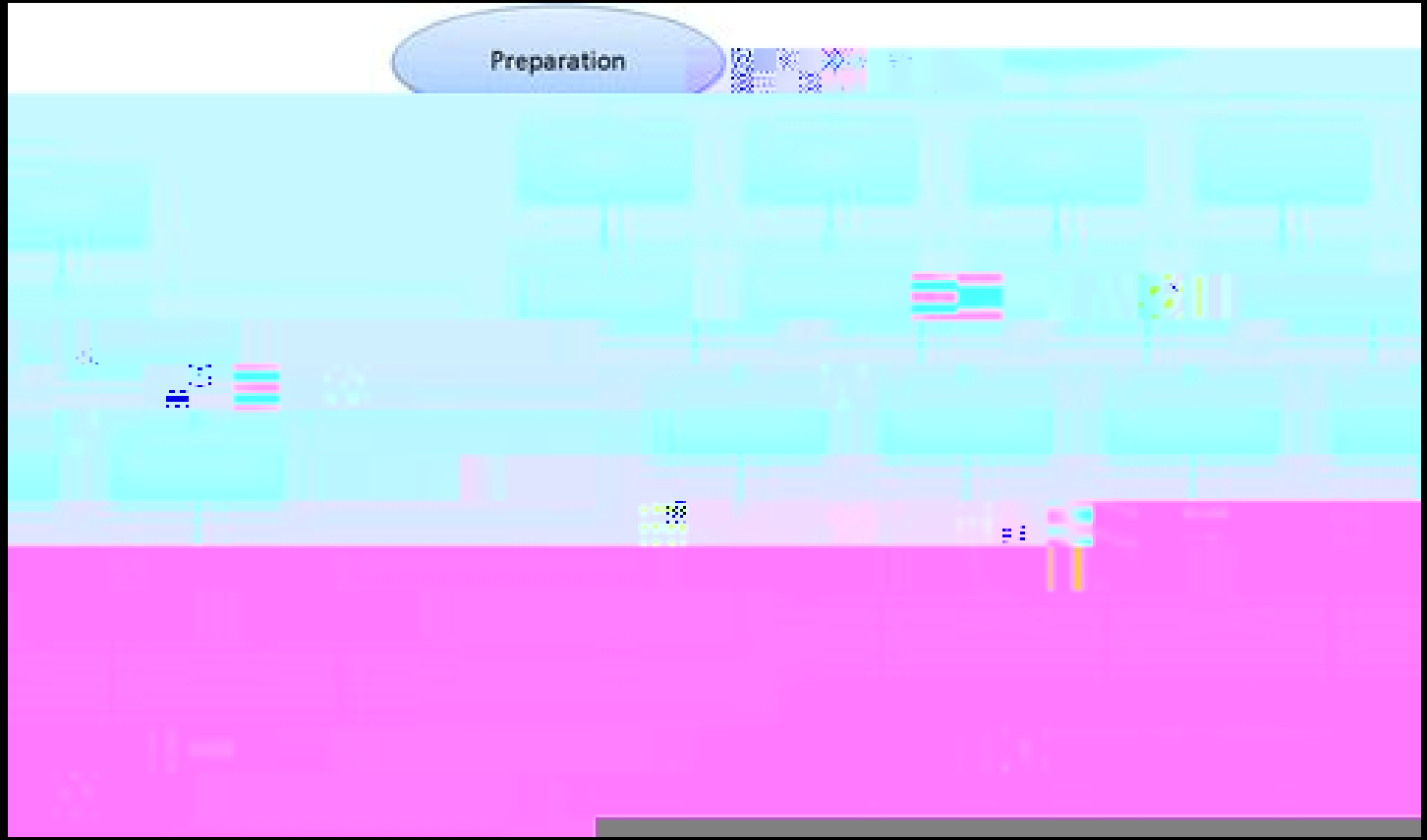
FabSim: an approach to mitigate Small Effort



Simple commands

fab archer cold	Compile the HemeLB code on ARCHER.
fab <machine> <code_name>: <config_name>	Run <code_name> with <config> on <machine_name>.
fab <machine> fetch_results	Fetch results from the runs from <machine_name>.
fab bluejoule lammps:h2osystem,\ cores=128,label=validation	Run LAMMPS on BlueJoule to

FabSim example



Source: Wan et al., 2015.

Thank you for your time

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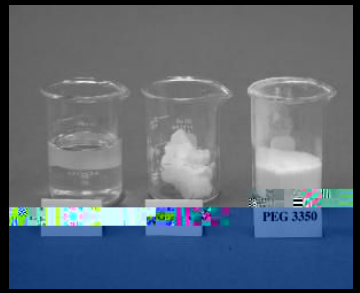
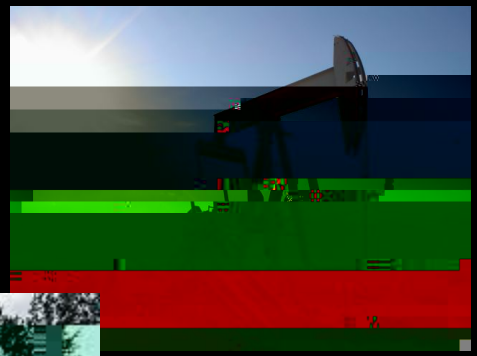


Clay

Multiscale applications: Clay-polymer nanocomposites

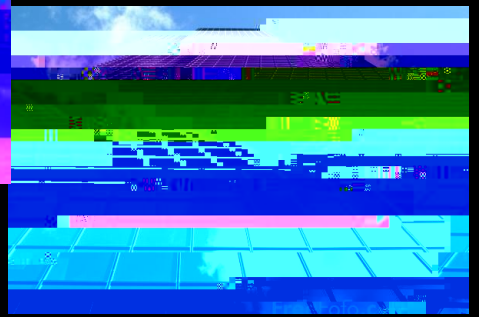
Aim: Develop quantitative coarse-grained models of clay-polymer nanocomposites.
Uses:

- Predict thermodynamically favourable states.
- Predict elasticity.



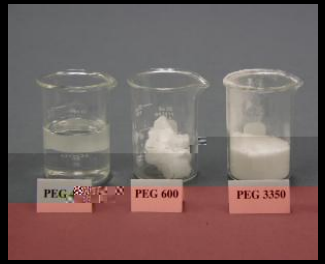
We require:

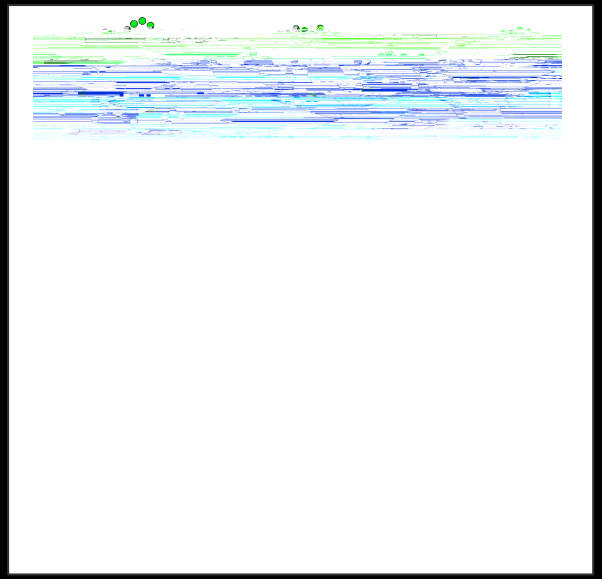
- Accurate potentials.
- Realistic structures.
- Representative time scales.



Suter, Groen and Coveney, Adv. Mat. 27 (6) 966-984, 2015.
Suter, Groen and Coveney, Nano Letters (ASAP), 2015.

Nanocomposites



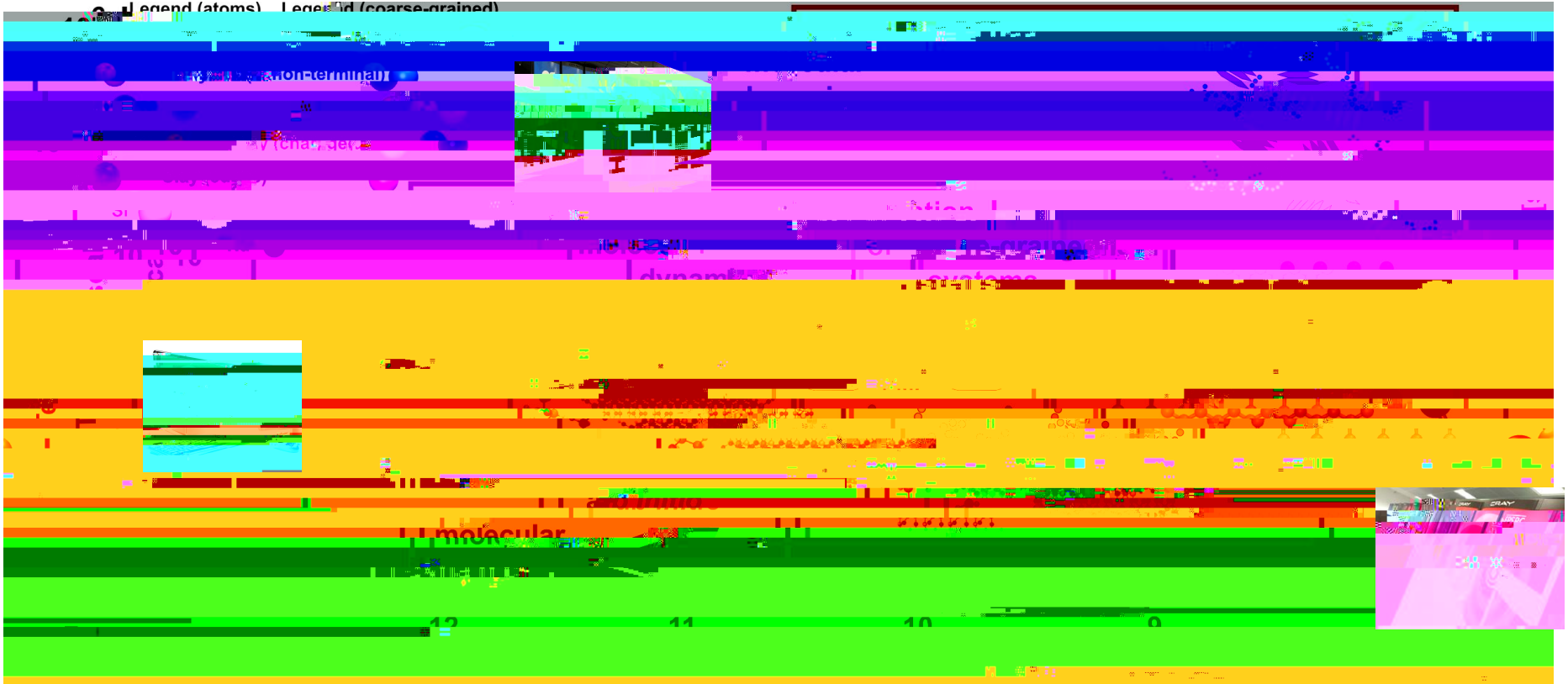


What we can do with single scale models

Suter et al., 2009

Sinsawat et al., 2003

Our multiscale approach



Future Work