

UNIVERSITY OF ILLINOIS  
AT URBANA-CHAMPAIGN

Department of Computer Science

1304 West Springfield Avenue  
Urbana, IL 61801 USA



December 22, 2003

Faculty Search Committee  
Department of Computer Science  
Indiana University

Dear Search Committee:

I am very pleased to write this recommendation on behalf of Wei WANG for a faculty position in your department.

Wei came to our Ph.D. program in 2000 from Ohio State where he had been a physics student involved in molecular dynamics. I hired him immediately as a research assistant for collaborative work with computational biophysicists. At Illinois he has done very well in coursework, with performance that is sometimes remarkable, e.g., first out of 29 graduate students in a networking course and 4th out of 43 students in Combinatorial Algorithms. He took the numerical computing Ph.D. qualifying exam in early 2001 while I was on leave at UCSD, and I was told that his performance on this exam was probably the best in the past decade.

Wei completed his M.S. thesis late in 2001 on the analysis of schemes for a certain type of stochastic differential equation (SDE). The topic of SDEs is more difficult than any usually encountered in scientific computing because it involves defining a probability measure on the space of continuous functions. The work was submitted for publication in spring 2002 and appeared this past August. It is the first result that I am aware of on the application of the "method" of modified equations to SDEs.

The topic of his Ph.D. thesis is the efficient calculation of polarizable force fields for molecular dynamics. It is now deemed desirable in the biomolecular simulation community to include the effects of polarizability. However, this increases the computing time by a factor of 6.5 for a simulation free of thermodynamics artifacts. Also the combination of dipoles with the particle-mesh Ewald algorithm significantly complicates the algorithm. Wei's aim is to use advanced and innovative numerical techniques to reduce the 550% penalty to less than 100%. Substantial progress to this goal has already

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been made, and a paper is now being prepared for publication. Wei has also done exploratory calculations that point to other techniques for obtaining additional significant improvements.

It is a joy to work with Wei. He is not only one of the most technically able graduate students in scientific computing but he has other qualities that bode well for his success. He has an enthusiasm for the subject and a charming sense of curiosity. He expresses himself well and is continually improving his English vocabulary. He takes the initiative to follow independent lines of inquiry, to search the literature, and to make contacts with established researchers. He is persistent and thorough in his research: to validate implementations of algorithms he does all that is possible to duplicate published results.

In sum, Wei works hard, and I believe his intelligence and enthusiasm will make him an excellent researcher and teacher.

Sincerely,

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